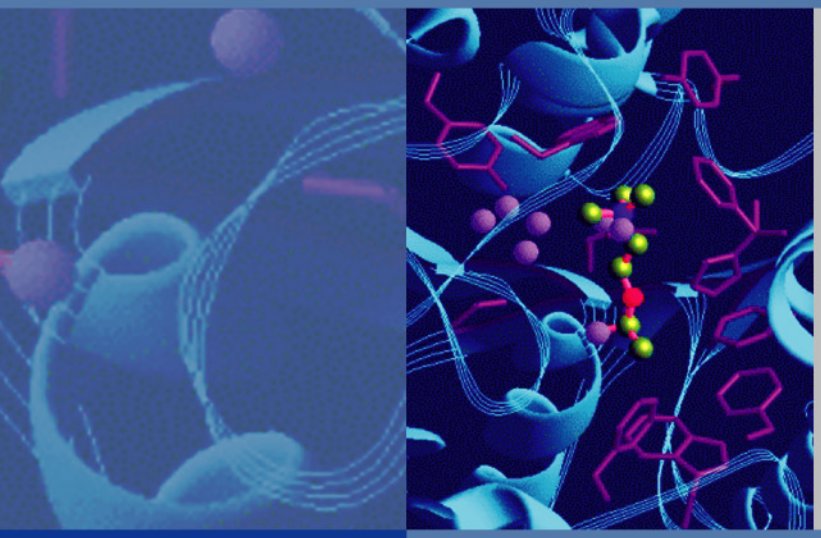

Xcalibur

QuickQuan

User Guide

XCALI-97195 Revision C July 2007

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Software Requirements: QuickQuan 2.1; Xcalibur 2.0.6 or 2.0.7; TSQ Quantum 1.5; Quan Devices 2.0; LC Devices 2.0.2 (includes Thermo PAL); Microsoft XP Service Pack 2; Microsoft Office 2003 or2007

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Preface

About This Guide

This user guide describes how to use QuickQuan™ 2.1 to perform high-throughput optimization and quantitative analysis of your compounds.

Related Documentation

The following QuickQuan manuals are available on the QuickQuan software CD as PDF files:

- *QuickQuan Installation Guide* describes how to install QuickQuan and register the database.
- *QuickQuan User Guide* describes how to use QuickQuan to perform high-throughput optimization and quantitative analysis of your compounds.
- *QuickQuan and Aria Quick Start* describes how to use QuickQuan with the Aria® OS software.

❖ To view the QuickQuan manuals

Go to **Start > Programs > Xcalibur > Manuals > QuickQuan**.

❖ To open the QuickQuan Help

From the QuickQuan window, choose **Help > QuickQuan Help**. To locate a particular topic, use the Help Contents, Index, or Search panes.

Special Notices

The guide includes the following types of special notices:

IMPORTANT Highlights information necessary to prevent damage to software, loss of data, or invalid test results; or may contain information that is critical for optimal performance of the system.

Note Highlights information of general interest.

Tip Helpful information that can make a task easier.

Contacting Us

There are several ways to contact Thermo Scientific.

❖ To contact Technical Support

Phone	800-685-9535
Fax	561-688-8736
E-mail	TechSupport.C+MS@thermofisher.com
Knowledge base	www.thermokb.com

Find software updates and utilities to download at www.mssupport.thermo.com.

❖ To contact Customer Service for ordering information

Phone	800-532-4752
Fax	561-688-8731
Web site	www.thermo.com/finnigan

❖ To suggest changes to documentation or to Help

- Fill out a reader survey online at www.thermo.com/lcms-techpubs.
- Send an e-mail message to the Technical Publications Editor at techpubs.finnigan-lcms@thermofisher.com.

Introduction

QuickQuan can optimize the selected reaction monitoring (SRM) transitions and tune parameters of multiple compounds, acquire chromatographic data, and generate quantitative results in a single analytical run. QuickQuan stores the compound optimization parameters in a database, so you can analyze the same compounds in multiple assays. You can use the database information to automatically generate the acquisition and post-acquisition methods for multiple analytical runs.

Contents

- QuickQuan Features
- QuickQuan Workflow

QuickQuan Features

QuickQuan does the following:

- Automates compound optimization and enables high-throughput compound optimization and acquisition.
- Provides a graphical interface for the layout of tune plates for compound optimization.
- Supports the importing of compound information and acquisition sequences.
- Uses a central database that supports access by local (acquisition) workstations and remote (analysis) workstations. The QuickQuan database can also support multiple instruments, which allows you to separate the optimization and the acquisition.
- Uses a Microsoft® Excel® worksheet to drive the acquisition, processing, and reporting of quantitative sequences using standard methods.
- Enables using an Excel macro to automatically generate custom calculations based on the post-acquisition results.
- Requires minimal input for rerunning complex assays.
- Enables you to bypass the chromatography column during optimization, and inject the samples directly into the ion source, which can speed up the optimization process (Thermo PAL® autosampler systems only).

QuickQuan Workflow

The first time you use QuickQuan, perform the following procedures. On subsequent uses, you can skip some of the steps if you plan to reuse the previous settings.

1. "Selecting QuickQuan Data Sources and Databases" on page 3
2. "Defining the Compounds and Drug Sets" on page 11
3. "Optimizing Your Compounds" on page 23 and "Viewing the Optimization Results" on page 36
4. "Acquiring the Sample Data" on page 43
5. "Reviewing the Results" on page 73

Note See the *QuickQuan 2.0 Installation Guide* for a description of how to install QuickQuan and register an ODBC database.

Selecting QuickQuan Data Sources and Databases

This chapter describes how to connect to the QuickQuan database via a data source.

Contents

- About the QuickQuan Database
- About the Data Source
- Selecting a File Data Source
- Creating a File Data Source

About the QuickQuan Database

QuickQuan stores compound information used for both compound optimization and data acquisition in a central database that supports access by local (acquisition) workstations and remote (analysis) workstations. The QuickQuan database can also support multiple instruments, which allows you to separate the optimization and the acquisition.

QuickQuan uses drug sets, which are groups of one or more compounds, to define which compounds to use for each sequence of samples in an assay or which compounds to optimize. Each database contains tables of information about the compounds and drug sets.

QuickQuan automatically writes the optimization data (polarity, parent and product ion masses, collision energy, and Q1 peak width) for each optimized compound to the database.

For a high-throughput acquisition run, QuickQuan uses the information stored in the specified database to build methods to analyze and process the data, and to provide reports on the analysis.

Note QuickQuan automatically opens the last used database. If you want to use this database, you can skip this chapter and go on to Chapter 3, "Defining the Compounds and Drug Sets."

Note To register the QuickQuan database, refer to the *QuickQuan Installation Guide*.

About the Data Source

A data source is a connection to a database. Typically, you create a separate data source connection for each database.

A data source name (DSN) is the logical name that the Open Database Connectivity (ODBC) uses to refer to the drive and other information that are required to access data.

Databases can have several general configurations. The QuickQuan database is typically configured as a file data source. This is the most flexible format for the database and can be used on a single computer or by several computers over a network.

Selecting a File Data Source

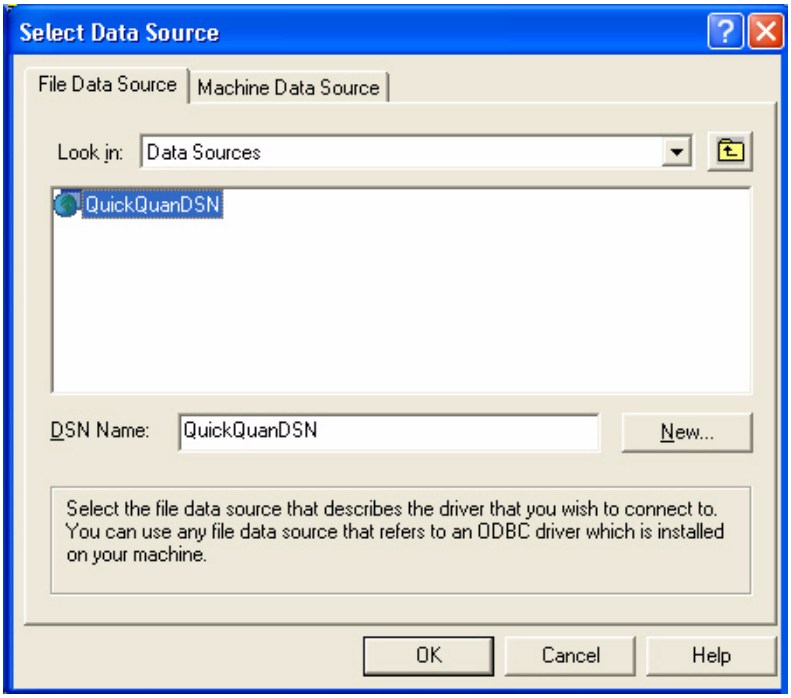
QuickQuan automatically opens the last used data source. You must select a data source in the following instances:

- At the first use of QuickQuan on your system
- If you want to change the data source for the current QuickQuan session

❖ To select a file data source

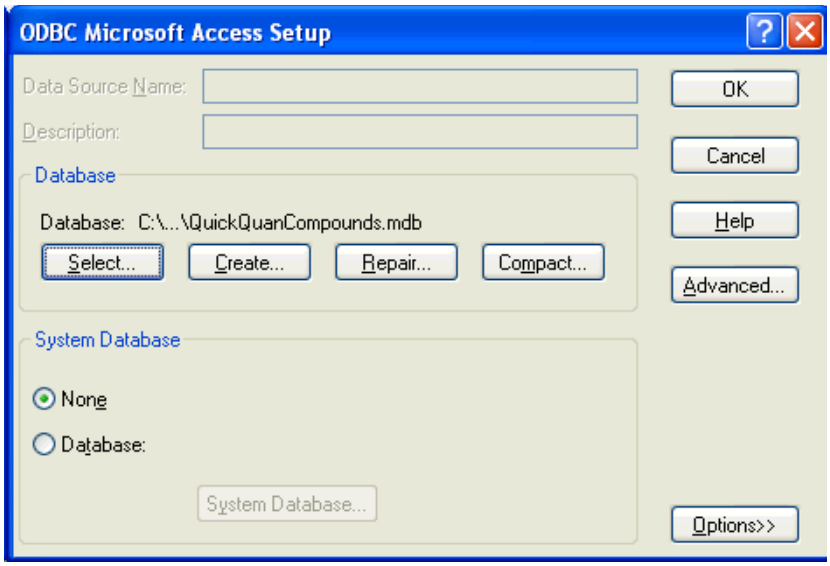
1. In the QuickQuan window, choose **File > Open Database**. The Select Data Source dialog box appears.
2. On the File Data Source page, select a file data source. See Figure 1.

Figure 1. Select Data Source dialog box, showing the file data source


Select Data Source
File Data Source
Machine Data Source
Look in:
Data Sources
QuickQuanDSN
DSN Name:
QuickQuanDSN
New...
Select the file data source that describes the driver that you wish to connect to. You can use any file data source that refers to an ODBC driver which is installed on your machine.
OK
Cancel
Help

3. Click **OK**, the ODBC Microsoft Access Setup dialog box appears.

Figure 2. ODBC Microsoft Access Setup dialog box



4. In the Database area, verify that the correct database name appears, for example, QuickQuanCompounds.mdb.

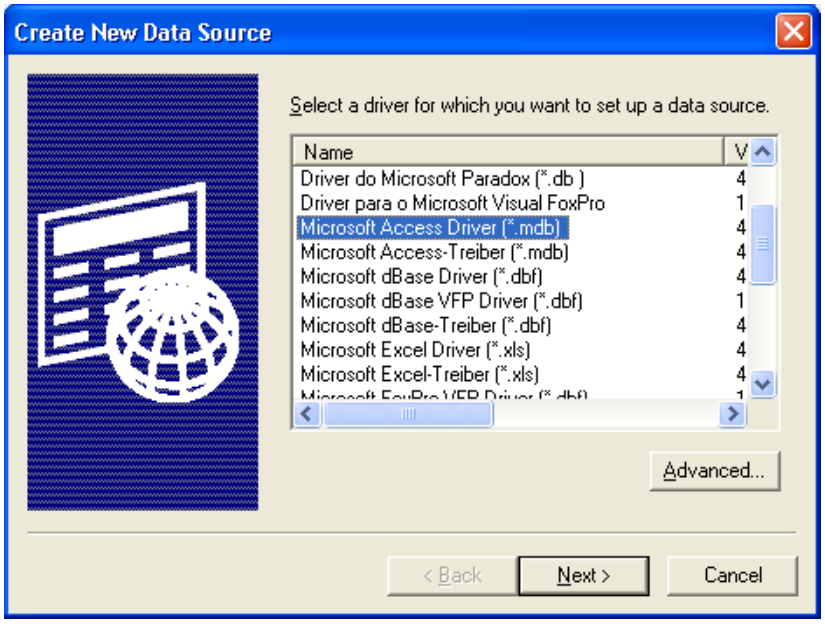
5. Click **OK** to close the dialog box.

Creating a File Data Source

❖ To create a new file data source

1. In the QuickQuan window, choose **File > Open Database**. The Select Data Source dialog box appears. See Figure 1.
2. On the File Data Source page, click **New**. The Create New Data Source wizard appears. See Figure 3.

Figure 3. Create New Data Source wizard – select driver list

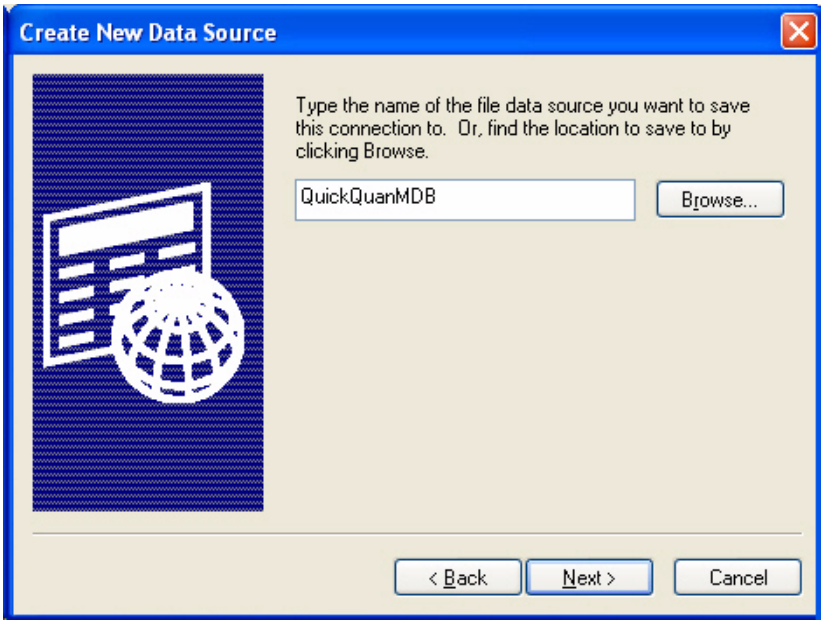


3. Select **Microsoft Access Driver (.mdb)** from the list of drivers, and then click **Next**.

Note If your site uses an Oracle® database, select an appropriate Oracle driver. Contact your local Oracle administrator for details on how to configure QuickQuan for an Oracle database.

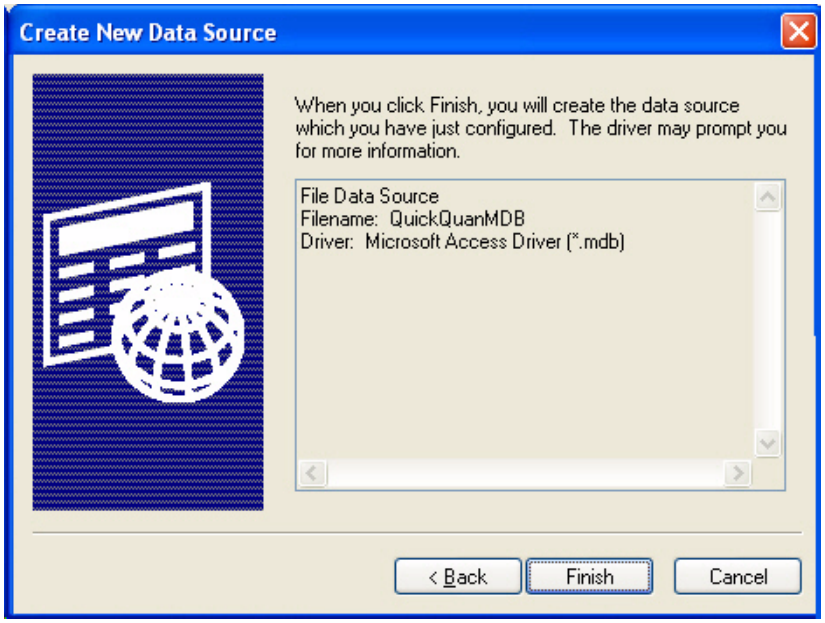
4. In the name box (Figure 4), type your data source name, for example, **QuickQuanMDB**. Click **Next**.

Figure 4. Create New Data Source wizard – name data source box


Create New Data Source
Type the name of the file data source you want to save this connection to. Or, find the location to save to by clicking Browse.
QuickQuanMDB
Browse...
< Back
Next >
Cancel

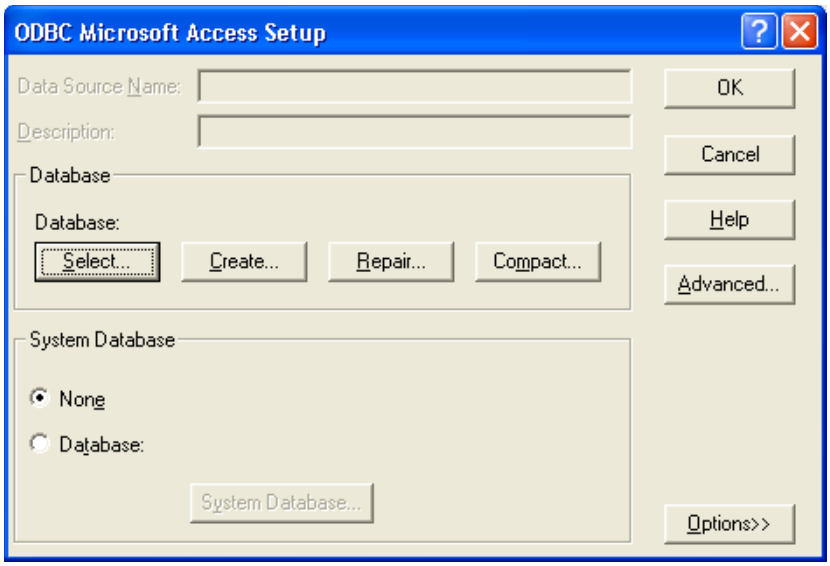
5. Verify that the file name of the new data source appears in the file data source box (Figure 5).

Figure 5. Create New Data Source wizard – Finish page


Create New Data Source
When you click Finish, you will create the data source which you have just configured. The driver may prompt you for more information.
File Data Source
Filename: QuickQuanMDB
Driver: Microsoft Access Driver (*.mdb)
< Back
Finish
Cancel

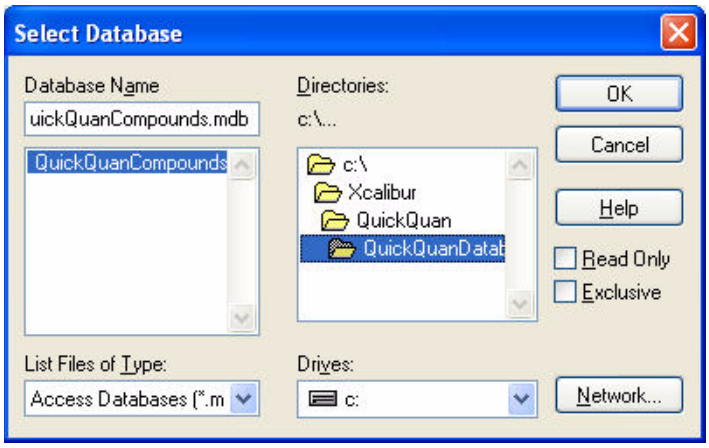
6. Click **Finish**. The software creates the file data source and then displays the ODBC Microsoft Access Setup dialog box (Figure 6).

Figure 6. ODBC Microsoft Access Setup dialog box



7. Click **Select**. The Select Database dialog box appears (Figure 7).

Figure 7. Select Database dialog box



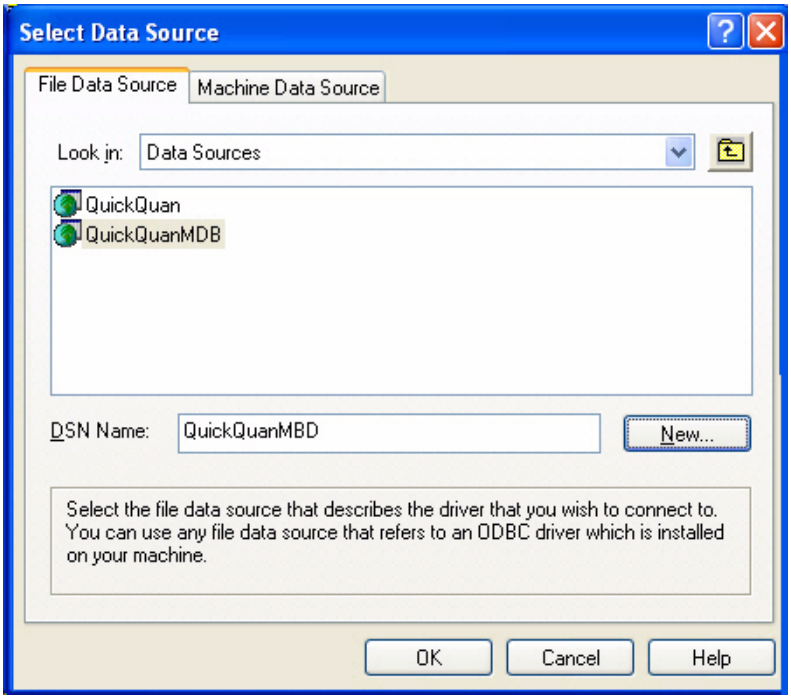
8. In the Directories box, browse to and select the **QuickQuanDatabase** folder. By default, the installation software places a QuickQuan database in the following folder:

   C:\Xcalibur\QuickQuan\QuickQuanDatabase

9. In the Database Name list, select the file **QuickQuanCompounds.mdb,** and then click **OK**.

10. Click **OK** to close the ODBC Microsoft Access Setup dialog box. The new data source, QuickQuan, appears in the Select Data Source dialog box. See Figure 8.

Figure 8. Select Data Source dialog box, showing the file data source


Select Data Source
File Data Source
Machine Data Source
Look in:
Data Sources
QuickQuan
QuickQuanMDB
DSN Name:
QuickQuanMBD
New...
Select the file data source that describes the driver that you wish to connect to. You can use any file data source that refers to an ODBC driver which is installed on your machine.
OK
Cancel
Help

11. Click **OK** to close the Select Data Source dialog box.

12. Click **OK** to close the ODBC Microsoft Access Setup dialog box.

Defining the Compounds and Drug Sets

This chapter describes how to assign compounds to drug sets within the database. A drug set can contain one or several compounds depending on the assay being run. You can create a multicompound drug set to facilitate simultaneous optimization and analysis of several analytes in the same sample. A cassette dosing experiment is one example of an assay where multicomponent drug sets are helpful.

Contents

- Defining the Compounds in the Database
- Defining the Drug Sets in the Database
- Viewing Compound and Drug Set Data

Defining the Compounds in the Database

The QuickQuan database must contain the compound information for the compounds in your QuickQuan experiments. You use the Add Compounds dialog box to manage the compound information stored in the database.

❖ To open the Add Compounds dialog box

In the QuickQuan navigation pane, click **Compounds**, and then click **Add Compounds**. The Add Compounds dialog box appears. See Figure 9 and Figure 10.

Use the following procedures to manage the compound information:

- "Manually Adding or Editing Compounds" on page 14
- "Importing Compounds Using a Text File" on page 14
- "Deleting Compounds " on page 17

Figure 9. Opening the Add Compounds dialog box

Click **Compounds**, and then click **Add Compounds**.

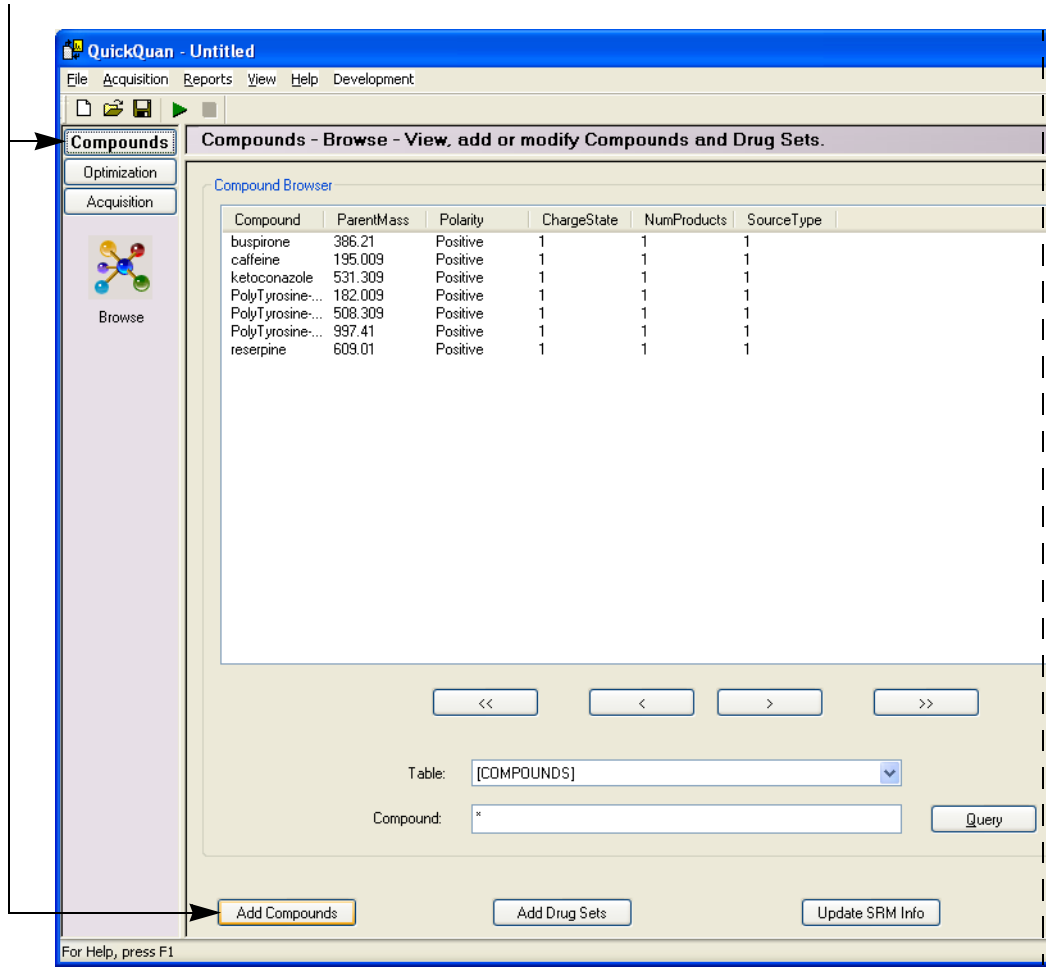
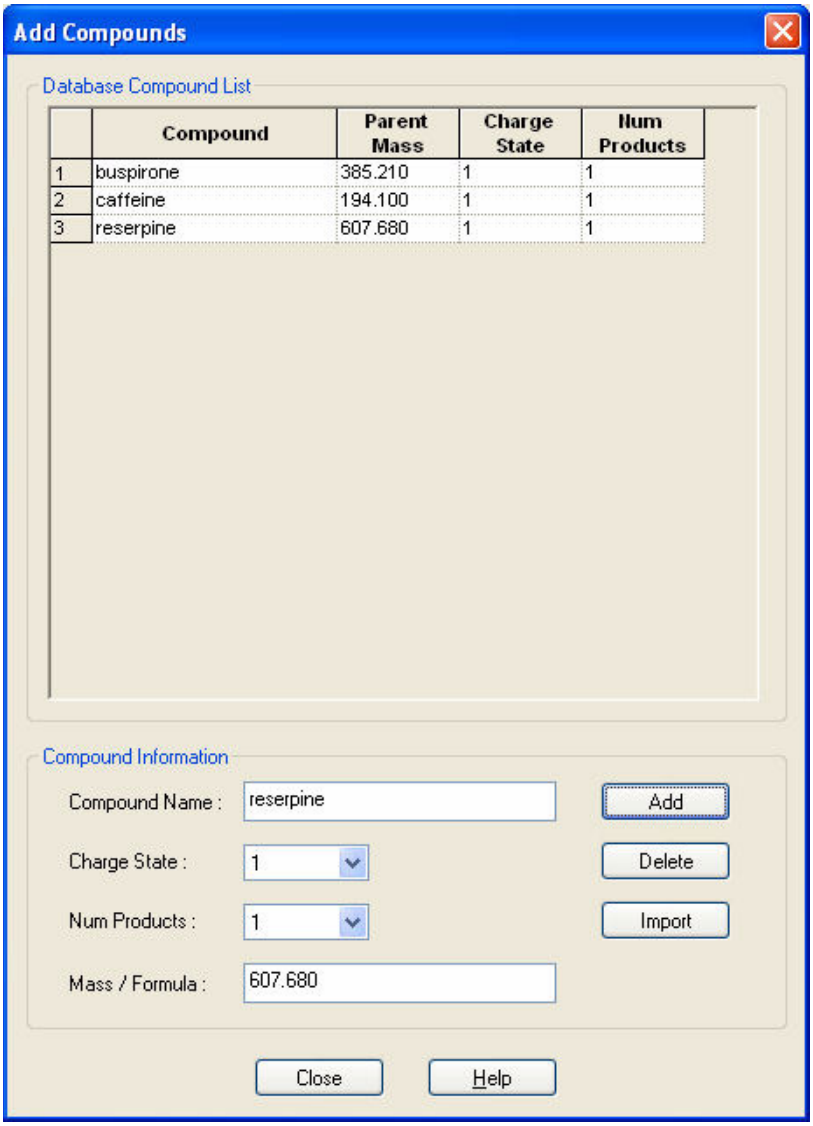


Figure 10. Add Compounds dialog box



Manually Adding or Editing Compounds

To add the compound information in the Add Compounds dialog box, add the information manually using the following procedure, or see "Importing Compounds Using a Text File" on page 14.

❖ **To add or edit compounds in a QuickQuan database**

1. In the QuickQuan navigation pane, click **Compounds**, and then click **Add Compounds.** The Add Compounds dialog box appears.
2. In the Compound Name box, type the new compound name.

   If you are editing a compound, select the compound in the Database Compound List.
3. In the Charge State box, select a charge state.
4. In the Num Products box, select the number of product ions for QuickQuan to detect.
5. In the Mass/Formula box, type the monoisotopic mass or the molecular formula for the compound.

   For example, if you were adding reserpine, the monoisotopic mass would be 607.680 instead of 608.680.
6. Click **Add**.
7. To add additional compounds, repeat steps 2 to 6.
8. Click **Close**.

Importing Compounds Using a Text File

You can import the compound information from a text file (.txt) instead of entering the information manually. The text file must be in a specified format. You can find example files in the following folder:

\Xcalibur\QuickQuan\ImportFiles

Creating a Text File for Importing Compounds

The text file can include either of the following:

- Compounds with molecular weight only
- Compounds with a Formula/Mass index and either molecular formula or molecular weight

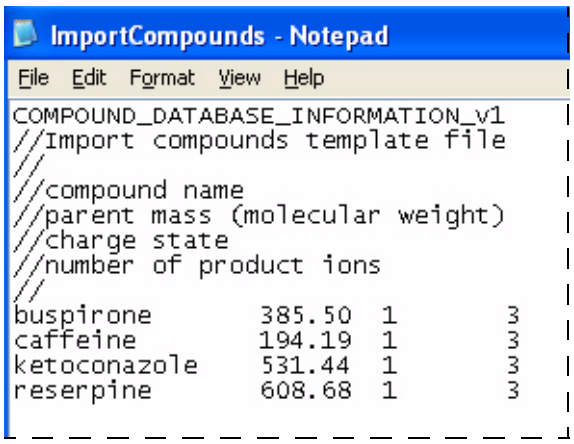
❖ To create a compound file with molecular weights only

1. Open a file in Microsoft Excel, Notepad, or any other software that allows you to create a tab-delimited text file with a .txt file extension.
2. In the first row of the text file, type the following text string:

   COMPOUND_DATABASE_INFORMATION_v1

   Figure 11 shows the file format for importing compounds with molecular weight only (no formulas).

   Figure 11. Compound file with molecular weights (no formulas)



3. (Optional) To include a comment in the file, use a double forward slash (//) at the start of the row. The software ignores any rows that begin with //.
4. In each row, enter the following fields. Use a separate row for each compound, and use a tab to separate each field in the row.

   compound name
   compound molecular weight
   charge state
   number of product ions to detect

5. Save the compound file as a .txt file.

❖ To create a compound file with molecular weights and formulas

1. Open a file in Microsoft Excel, Notepad, or any other software that allows you to create a tab-delimited text file with a .txt file extension.
2. In the first row of the file, type the following text string:

   COMPOUND_DATABASE_INFORMATION_v2

3. (Optional) To include a comment in the file, use a double forward slash (//) at the start of the row. The software ignores any rows that begin with //.

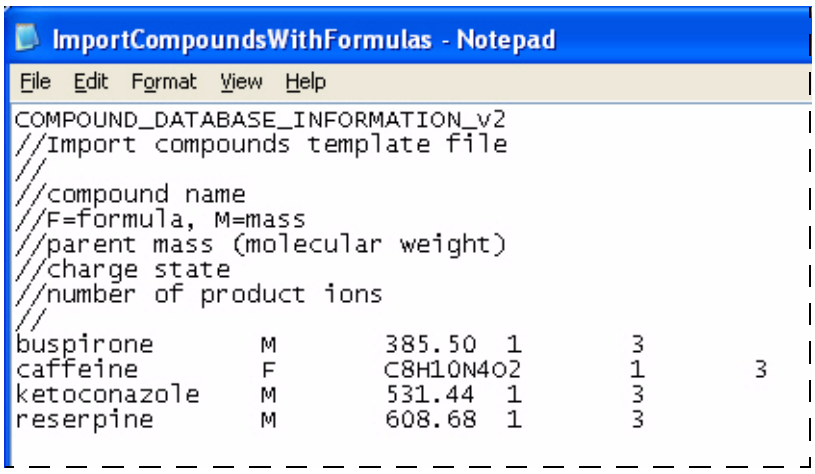
4. In each row, enter the following fields. Use a separate row for each compound, and use a tab to separate each field in the row.

   compound name
   formula (F) or mass (M) index
   compound molecular weight or molecular formula
   charge state
   number of product ions to detect

5. Save the compound file as a .txt file.

Figure 12 shows the file format for importing compounds with both molecular weights and formulas.

Figure 12. Compound file with both molecular weights and formulas



Importing the Compounds Text File

❖ To import the compound file to the QuickQuan database

1. In the QuickQuan navigation pane, click **Compounds**, and then click **Add Compounds**. The Add Compounds dialog box appears (Figure 10).
2. Click **Import**.
3. Click **Yes** when the confirmation message appears.
4. In the Open dialog box, select the file you want to import, and then click **Open**. The compounds appear in the Database Compound List.
5. Click **Close**.

Deleting Compounds

❖ **To delete compounds from a QuickQuan database**

1. In the QuickQuan navigation pane, click **Compounds**, and then click **Add Compounds.** The Add Compounds dialog box appears.
2. In the Database Compound list, click the compound, and then click **Delete**. Repeat this step for any other compounds you want to delete.
3. When you have finished deleting compounds, click **Close**.

Defining the Drug Sets in the Database

In QuickQuan, compounds are grouped together in drug sets. The tune plate and the acquisition assay both use drug sets to define the compounds associated with one another for each tuning well or acquisition sequence. If you do not specify a drug set for a compound, QuickQuan adds a drug set containing just that compound to the database.

Note Up to 10 compounds can be associated with a single drug set.

Use the following procedures to manage the drug sets:

- "Adding Drug Sets Manually " on page 17
- "Importing Drug Sets Using a Text File" on page 19
- "Deleting Drug Sets " on page 20

Adding Drug Sets Manually

You can create drug sets manually and edit the compounds included in a given drug set.

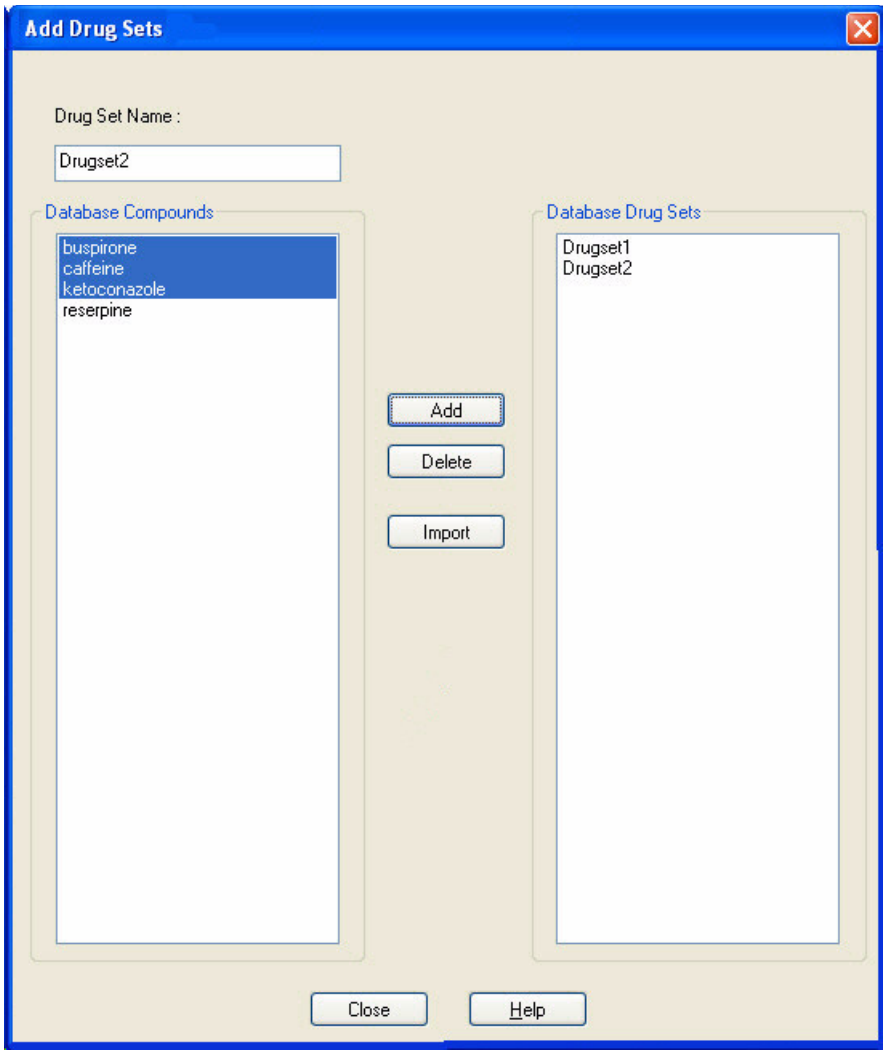
❖ **To create a drug set in a QuickQuan database**

1. In the QuickQuan navigation pane, click **Compounds**.
2. In the Compounds Browse view, click **Add Drug Sets**. The Add Drug Sets dialog box appears (Figure 13).
3. In the Drug Set Name box, type the name.
4. In the Database Compounds list, click each compound you want to add to the new drug set.
5. Click **Add**. QuickQuan adds the selected compounds to the drug set, and the drug set name appears in the Database Drug Sets list.

❖ To add compounds to a drug set

1. In the Database Drug Sets list, select the drug set name.
2. In the Database Compounds list, click each compound you want to add to the drug set.
3. Click **Add**. QuickQuan adds the selected compounds to the drug set.
4. Click **Close**.

Figure 13. Add Drug Sets dialog box



❖ To remove compounds from a drug set

1. In the Database Drug Sets list, select the drug set name.
2. In the Database Compounds list, click each compound you want to remove from the drug set.
3. Click **Delete**.
4. Click **Close**.

Importing Drug Sets Using a Text File

You can import the drug set information from a text file (.txt) into a QuickQuan database. The text file must be in a specified format. You can find an example file in the following folder:

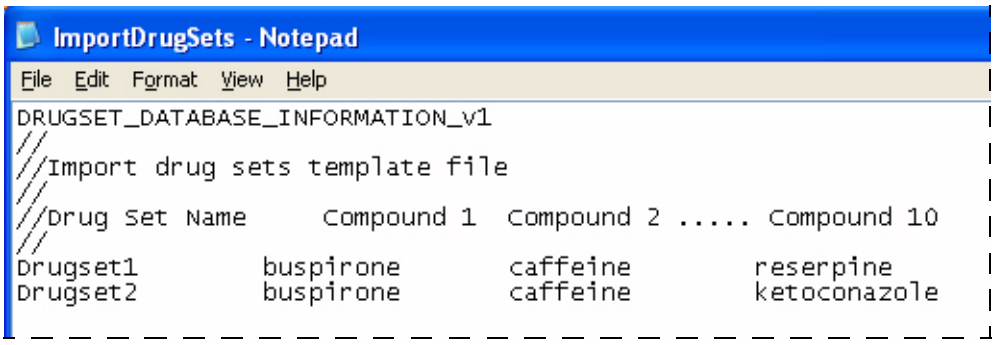
\Xcalibur\QuickQuan\ImportFiles

❖ To create a drug set file for importing

1. Open a file in Microsoft Excel, Notepad, or any of the software that allows you to create a tab-delimited text file (.txt file extension).
2. Enter the following string in the first row of a text file:

   DRUGSET_DATABASE_INFORMATION_v1
3. (Optional) To include a comment in the file, use a double forward slash (//) at the start of the row. The software ignores any rows that begin with //.
4. In each row, enter the drug set name followed by up to 10 compound names. Use a separate row for each drug set and use a tab to separate each field in the row. Figure 14 shows the file format for importing drug set names.
5. Save the file as a .txt file.

Figure 14. Drug set names file created in Excel and saved to a .txt file



❖ To import the drug set file

1. In the QuickQuan navigation pane, click **Compounds**, and then click **Add Drug Sets**. The Add Drug Sets dialog box appears (Figure 13).
2. Click **Import**.
3. Click **Yes** when the confirmation message appears.
4. In the Open dialog box, select the drug set file you want to import, and then click **Open**. The drug sets appear in the Database Drug Sets list.
5. Click **Close** to close the dialog box.

Deleting Drug Sets

❖ To delete drug sets from the QuickQuan database

1. In the QuickQuan navigation pane, click **Compounds**, and then click **Add Drug Sets**. The Add Drug Sets dialog box appears.
2. In the Database Drug Set List, click the drug set, and then click **Delete**. Repeat this step for any other drug set you want to delete.
3. When you have finished deleting drug sets, click **Close**.

Viewing Compound and Drug Set Data

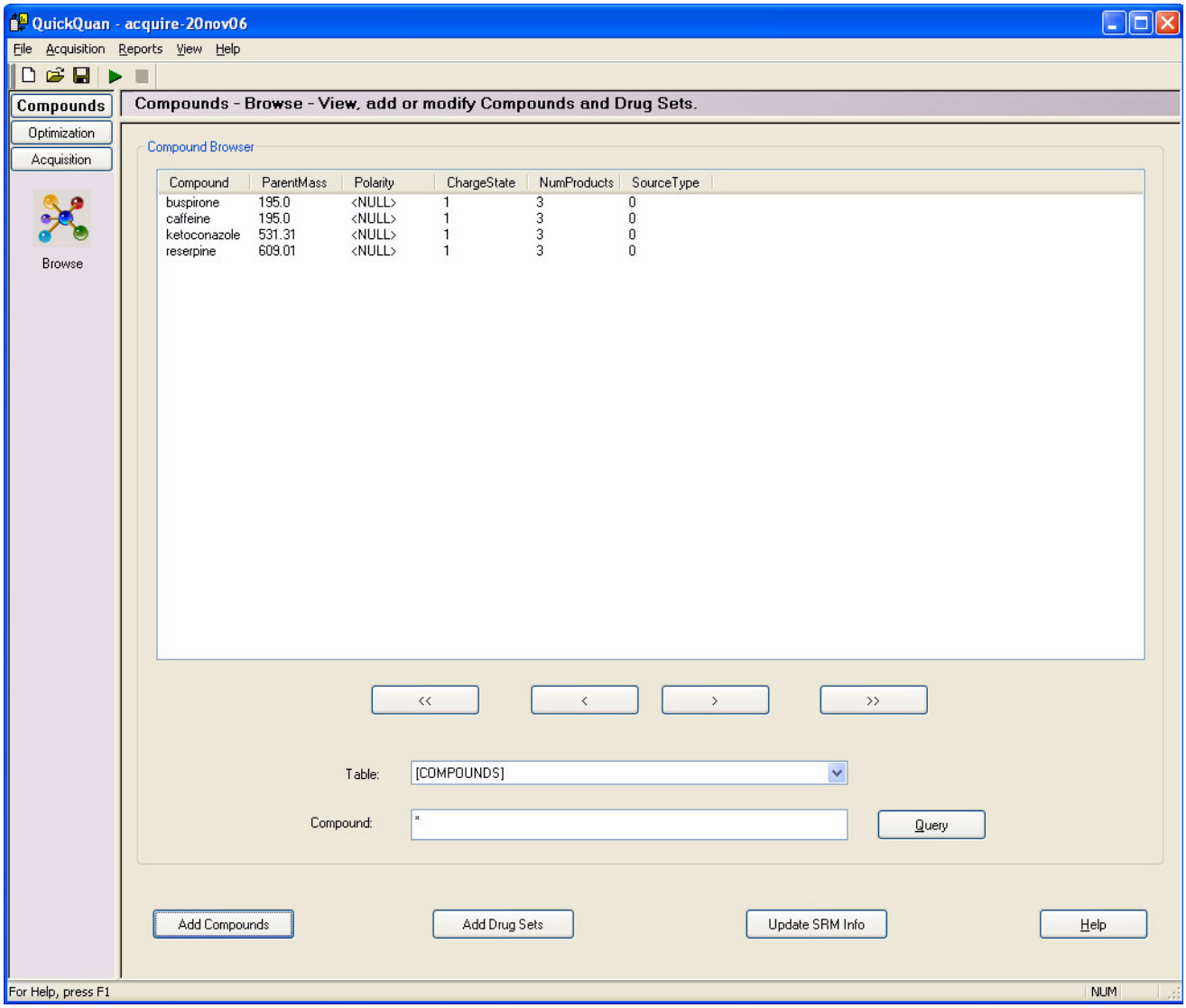
Use the Compounds Browse view to view the contents of the database tables for the currently opened QuickQuan database. You can also enter SQL query commands to filter the data in the tables.

For more details on the Compounds Browse view, see "Compounds Browse View" on page 85.

❖ To view compounds with the Compound – Browse view

1. Click **Compounds** to display the Compounds Browse view.
2. In the Table box, select **[COMPOUNDS]**. The Compounds table appears. See Figure 15.
3. (Optional) If the table contains many rows and you want to move around in the table without having to scroll row by row, click the << , < , > , and >> buttons to change the view in the table.
4. (Optional) To use an SQL statement to filter the data, type the SQL statement in the Compound box, and then click **Query** to filter the data.

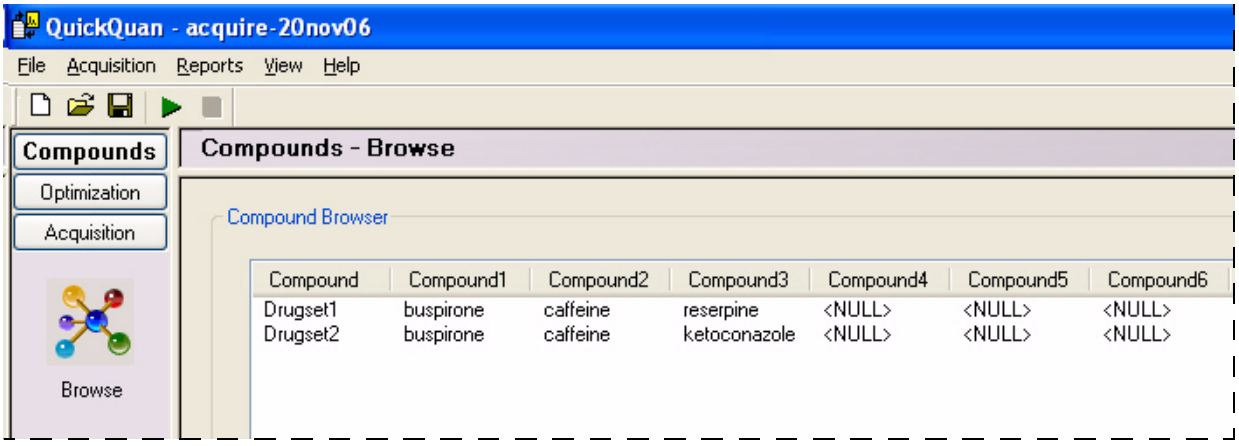
Figure 15. Compounds Browse view, showing the compounds table



❖ To view drug sets with the Compounds Browse view

1. In the Table box, select **[DRUGSETNAME]**. The Drug Set table appears. See Figure 16.
2. (Optional) If the table contains many rows and you want to move around in the table without having to scroll row by row, click the << , < , > , and >> buttons to change the view in the table.

Figure 16. Compounds Browse view, showing the Drug Set table



Optimizing Your Compounds

This chapter describes how to automatically optimize the tune and SRM parameters for all the compounds defined in the tune plate.

Contents

- Understanding the Compound Optimization Process
- Setting Up for Optimization
- Running the Optimization
- Viewing the Optimization Results
- Updating SRM Information

Before you set up the tune plate information, add compounds and drug sets to your selected database as described in "Defining the Compounds and Drug Sets" on page 11.

Understanding the Compound Optimization Process

You assign a drug set to each well in the tune plate. QuickQuan passes the compound information from the drug set to the TSQ® Quantum tune application in real-time, and then monitors the status of each compound during the optimization. The data returned from the optimization is added to the QuickQuan database.

The optimization data for each compound includes the following:

- Polarity
- Precursor ion mass
- Product ion masses
- Collision energy
- Q1 peak width
- Tube lens voltage
- Product ion intensity

Tip QuickQuan uses instrument methods for optimization that differ from those for acquisition. If your system includes a Thermo PAL autosampler with multiple injection ports, multiple valves, and a stream selector, you can use QuickQuan to bypass the chromatography (LC) column during optimization, speeding up the optimization process. See "Bypassing the LC Column and the Dual-Pump, Dual-Column Configuration" on page 81.

If you are using the LC column, and the tune operation times out before the compounds have been tuned, use a longer delay for the divert valve setting.

Setting Up for Optimization

IMPORTANT Before you can set up for optimization, you must have configured an autosampler. To configure an autosampler, see "Configuring and Setting Up Instruments" on page 79.

To set up for optimization, perform the following procedures:

- "Specifying Tune and Method Files and Optimization Settings" on page 25

  Or, you can reuse the settings from a previous optimization. See "Reusing Optimization Settings" on page 24.

- "Setting Up the Tune Plate for Compound Optimization" on page 27

Reusing Optimization Settings

You can reuse the settings from an acquisition (.aql file) that you have already created in QuickQuan. The .aql file contains the configuration settings, acquisition settings, compound optimization information, assay layout, and the template information.

❖ To reuse the settings in an .aql file

1. In the QuickQuan window, choose **File > Open**.
2. In the Open dialog box, select the .aql file, and then click **Open**. For example, open the following:

   \Xcalibur\examples\QuickQuan\SampleSet\optimization template.aql

3. Verify the optimization settings in the Optimization Setup view. See "Specifying Tune and Method Files and Optimization Settings" on page 25.

Specifying Tune and Method Files and Optimization Settings

You specify the tune and method files, optimization settings, and output path in the Optimization Setup view.

❖ To display the Optimization Setup view

In the QuickQuan navigation pane, click **Optimization**, and then click **Setup**.

❖ To specify method files, optimization settings, tune plate settings, and output path

1. In the Tune and Method Files area, specify the file or folder path for each of the following.

   To select a file, click the ... button for the item, and then select the location.

   a. In the Tune File box, specify the generic tune file. For an example, select

      C:\Xcalibur\QuickQuan\Templates\tune template.TSQTune.

      IMPORTANT Tune parameters are instrument parameters that affect the intensity of the ion signal. You must specify a generic tune file that corresponds to the type of experiment you are performing, for example ESI high-flow. During tune optimization, QuickQuan determines additional settings, such as polarity, tube lens voltage, parent and product ion masses, Q1 peak width, and collision energy. These settings, which maximize the ion signal for your compounds, are added to the settings in the generic tune file.

   b. In the Tune Pos. LC Method box, specify the method file that contains the LC settings for a positive polarity tune optimization. For an example, select

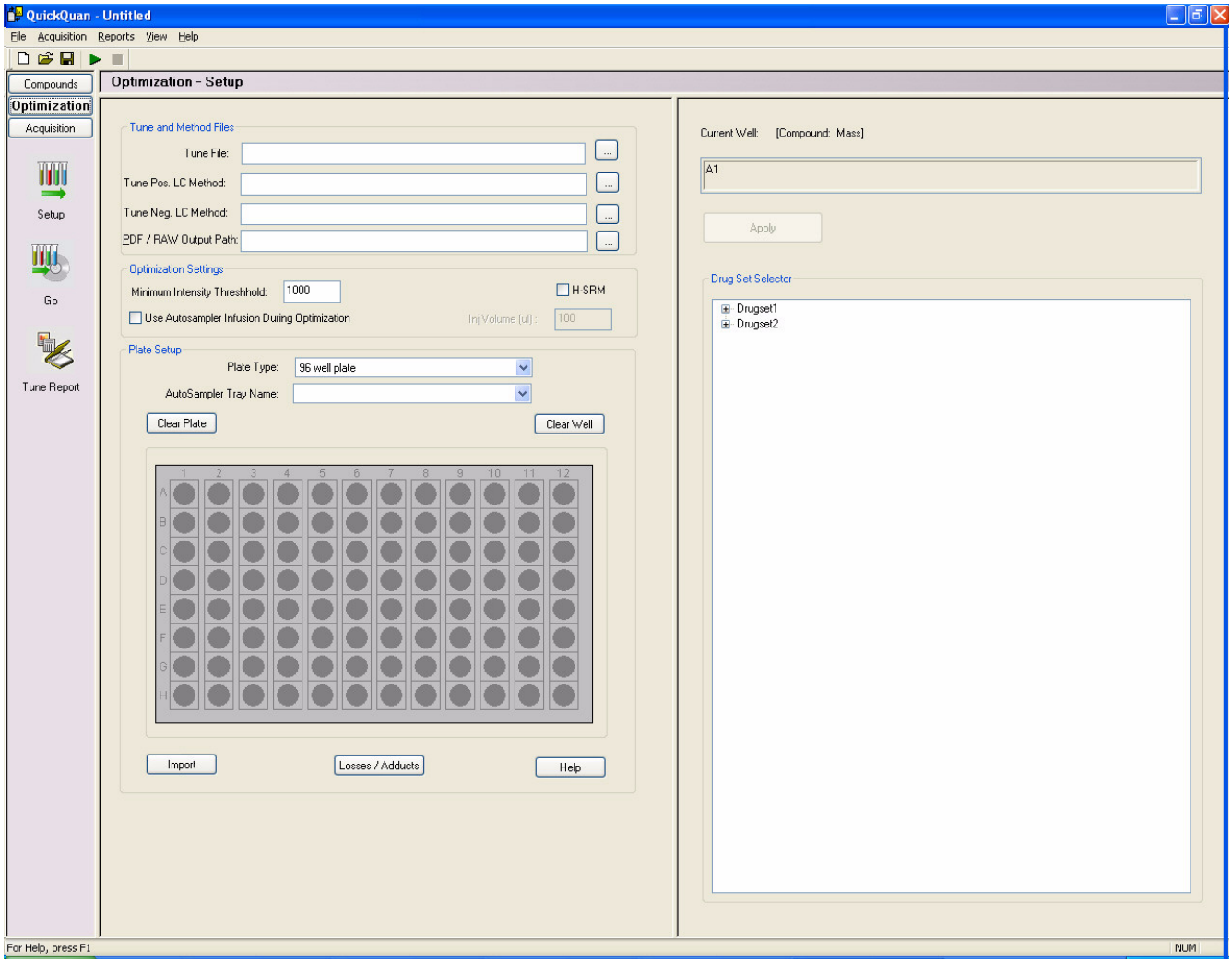
      C:\Xcalibur\QuickQuan\Templates\Tune_LC_Pos.meth.

   c. In the Tune Neg. LC Method box, specify the method file that contains the LC settings for a negative polarity tune optimization. For an example, select

      C:\Xcalibur\QuickQuan\Templates\Tune_LC_Neg.meth.

   d. In the PDF / RAW Output Path box, enter the folder path for the export folder.

Figure 17. Optimization Setup view



2. In the Minimum Intensity Threshold box, type the minimum intensity threshold for the product ions.
3. (Optional) Select the **H-SRM** check box to specify tuning for H-SRM (precursor ion peak width = 0.2 amu).
4. (Optional) To specify a flow injection (infusion) of a single sample for optimization, select the **Use Autosampler Infusion During Optimization** check box, and then type the sample amount to inject for each compound in the Inj Volume box.

   Or, to perform multiple injections of each sample for the optimization run, clear the **Use Autosampler Infusion During Optimization** check box.
5. In the Plate Type list, select the autosampler plate type to be used for this optimization.
6. In the Autosampler Tray Name box, select the name of the autosampler tray to be used for this optimization.

Setting Up the Tune Plate for Compound Optimization

QuickQuan uses the compound information specified in a drug set to optimize all the compounds within the drug set. One drug set is assigned to each well of the plate. The tune plate can represent hundreds of compounds at a single time, each compound being optimized individually. You can arrange the drug sets within the tune plate in any desired layout.

❖ To set up the tune plate for compound optimization

1. Specify the drug sets in the tune plate by doing one of the following:
   - Use the tune plate graphic to add drug sets, one at a time. See "Using the Tune Plate Graphic to Add Drug Sets Manually ."
   - Import the tune plate information from a text file. See "Importing Tune Plate Information Using a Text File" on page 31.
2. (Optional) To select adducts or to disallow product ion losses that are not specific enough, click **Losses/Adducts**. In the Losses/Adducts dialog box, select the adducts to include and the product ion losses you want to disallow, and then click **OK**.

Using the Tune Plate Graphic to Add Drug Sets Manually

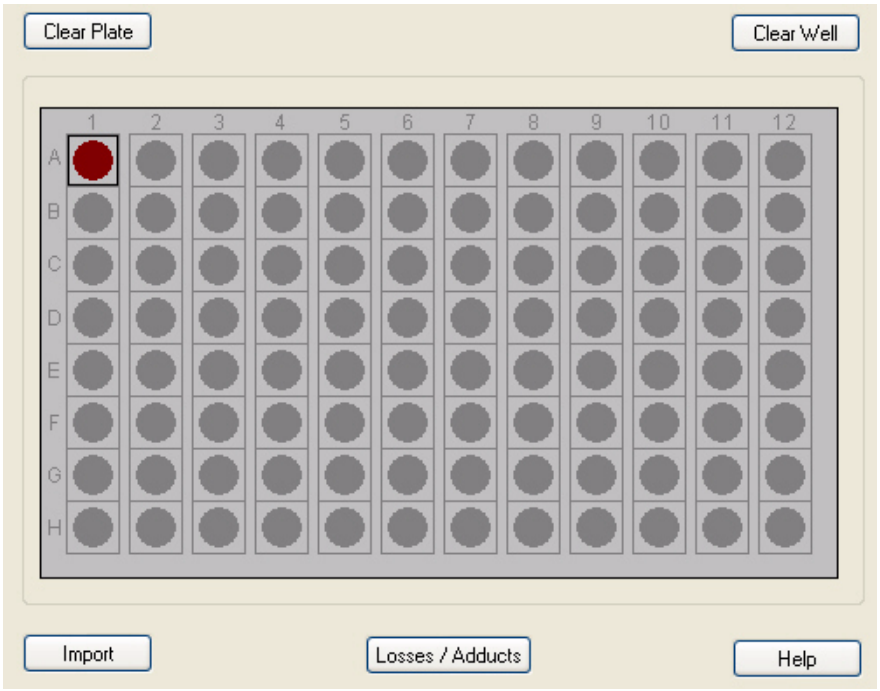
You set the injection order based on the order in which you add the drug sets to the tune plate graphic. For example, if you add the first compound to well position C2 and the second compound to A1, the first injection is taken from C2 and the second from A1, and so on.

❖ To add drug sets using the tune plate graphic

In the QuickQuan navigation pane, click **Optimization**, and then click **Setup**.

1. In the Optimization Setup view, click a well position in the tune plate graphic. See Figure 18.

Figure 18. Tune plate graphic

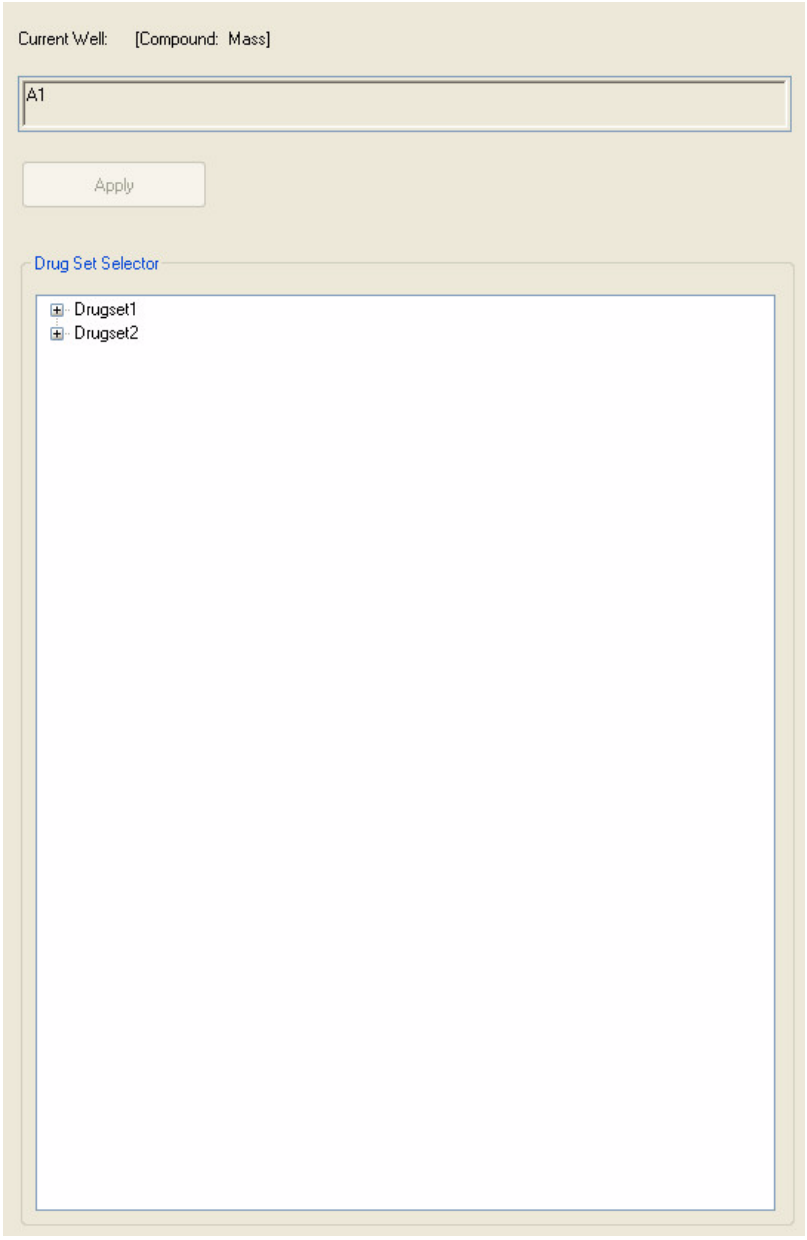


2. Select a drug set in the Drug Set Selector. See Figure 19.

   Notice that the selected well positions on the tune plate graphic are color-coded as follows:

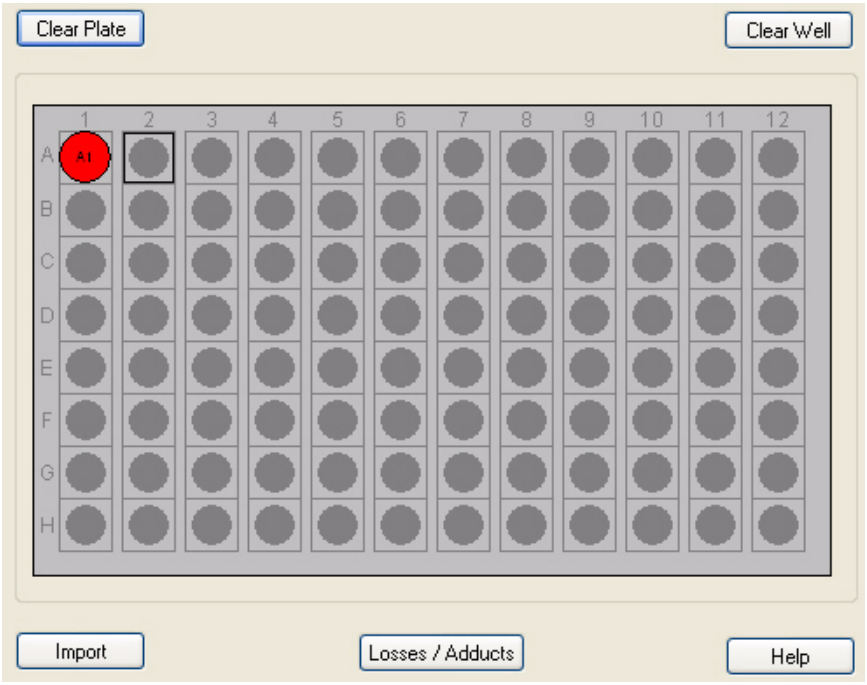
   - **Green:** All compounds in the well (drug set) have been optimized for the currently selected ion source.
   - **Yellow:** All compounds in the well have been optimized for an ionization source other than the currently selected ion source.
   - **Red:** At least one compound in the well has not been optimized.

Figure 19. Drug Set Selector and current well information



3. Click **Apply** to associate the drug set to the well. The tune plate in Figure 20 shows well A1 is red, indicating at least one unoptimized compound.
4. Repeat steps 1 to 3 for each well position.
5. Choose **File > Save**. QuickQuan saves the tune plate information in an .aql file.

Figure 20. Tune plate graphic, indicating unoptimized compounds in well position A1



Importing Tune Plate Information Using a Text File

You can import a text file (.txt) that contains all the tune plate information that you would otherwise enter manually using the tune plate graphic in the Optimization Setup view. When you import the file that contains all the tune plate information, QuickQuan adds the tune plate information to the database.

Creating a Tune Plate Information File

An example file for importing tune plate information is in the following folder:

\Xcalibur\QuickQuan\ImportFiles

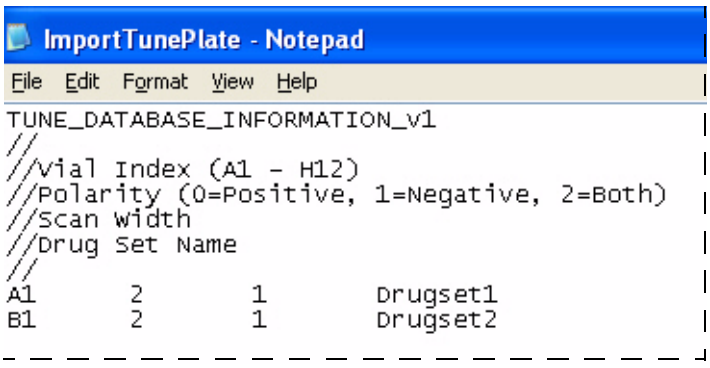
❖ To create a tune plate information file

1. Open a new file in Microsoft Excel, Notepad, or any other software that allows you to create a tab-delimited text file with a .txt file extension.
2. In the first row of the file, type the string: TUNE_DATABASE_INFORMATION_v1.
3. (Optional) To include a comment in the file, use a double forward slash (//) at the start of the row. The software ignores any rows that begin with //.
4. In each row, type the following fields. Use a separate row for each well, and use a tab to separate columns. Figure 21 shows an example.

   well index
   polarity
   scan width
   drug set name

5. Save the tune plate information file as a .txt file.

Figure 21. Tune plate information (.txt) file

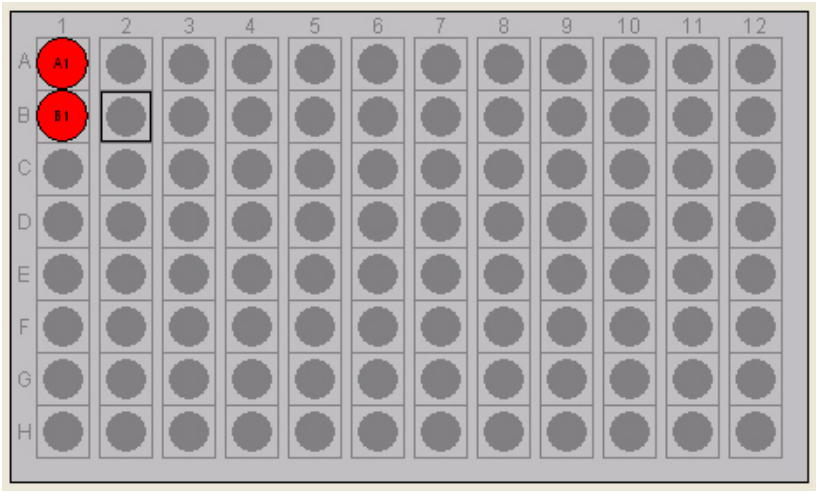


Importing the Tune Plate Information File

❖ **To import the tune plate information file**

1. In the Optimization Setup view, click **Import**. A message asks if you want the imported file to overwrite well information for existing well positions.
2. Click **Yes**. The Open dialog box appears.
3. In the Open dialog box, select the tune plate information file (.txt), and click **OK**. Figure 22 shows the tune plate graphic after importing information for wells A1 and B1.
4. Choose **File > Save**. QuickQuan saves the tune plate information in an .aql file.

Figure 22. Tune Plate graphic with samples in positions A1 and B1



Running the Optimization

After you set up the optimization, you can do either of the following:

- Run only the optimization per the following procedure.
- Acquire the data for an assay with real-time compound optimization. In this case, see "Acquiring the Sample Data" on page 43.

In either case, you can choose to use the information in the database or to force the optimization of the compounds to update the database.

❖ To display the Configuration Options dialog box

In the QuickQuan navigation pane, click **Optimization**, and then click **Go**.

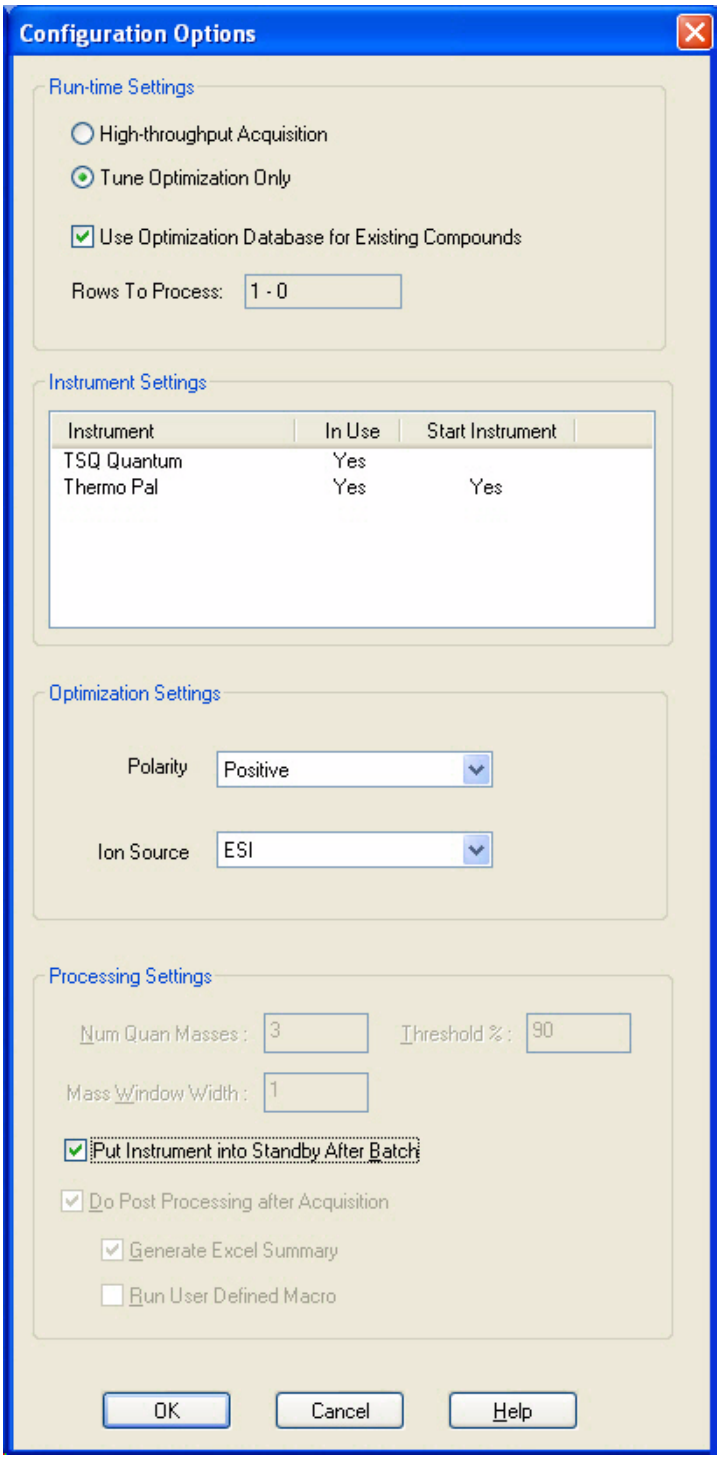
❖ To run the optimization only

1. In the Configuration Options dialog box, select the **Tune Optimization Only** option. See Figure 23.
2. (Optional) To use optimization information that is already in the database, select the **Use Optimization Database for Existing Compounds** check box. QuickQuan optimizes the compounds in the tune plate that have not been optimized.

   If the check box is cleared, QuickQuan optimizes all compounds that are in the tune plate.
3. In the Instrument Settings area, verify the following:
   a. The Instrument column lists only the required instruments. If the required instruments do not appear, update the Xcalibur instrument configuration per "Configuring and Setting Up Instruments" on page 79.
   b. The In Use column displays a **Yes** for each instrument. If necessary, click the **In Use** cell to toggle on or off the **Yes**.
   c. (Optional) The Start Instrument column displays **Yes** for the instrument that you want to initiate the run.

> **Note** Typically, the autosampler is selected to be the start instrument because it controls when a run starts. In this case, the In Use column displays a Yes for all instruments to be used for the sequence submission, including the autosampler. This means the instruments are awaiting a contact closure event to start operation. When this status has been achieved by all instruments used in the run, the start instrument initiates the run.

Figure 23. Configuration Options dialog box



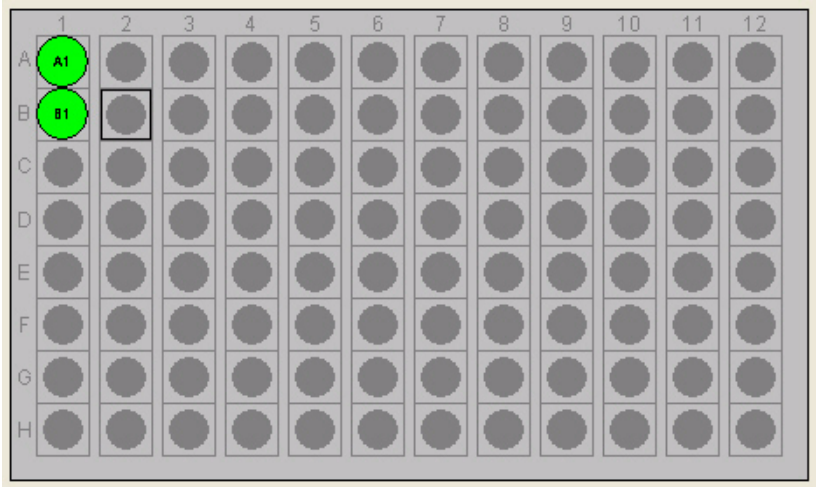
4. In the Optimization Settings area, select the following:
   a. **Polarity**: positive, negative, or both
   b. (Optional) **Ion source**: ESI, APCI, APPI, or H-ESI
5. Select the **Put Instrument Into Standby Mode After Batch** check box to set the devices to standby after the acquisition has finished.
6. Prepare to run the optimization.
   a. Open Xcalibur to the Real Time Plot view.
   b. In Xcalibur, verify that the instrument status is Ready to Download, and make sure the initial system parameters are within the acceptable ranges.
   c. Verify that the vessel holding the compounds for tuning is ready and in position. Verify the same for assay plates.
   d. Start Quantum EZ Tune.
7. In the Configuration Options dialog box, click **OK**. QuickQuan starts the optimization and displays the Optimization Status view.

Tip You can also view the status of the run in the EZ Tune Real Time Plot view.

8. After the optimization, verify that the compounds were optimized successfully.

Figure 24 shows a successful optimization in the Optimization Setup view.

Figure 24. Tune plate graphic showing optimized compounds



Viewing the Optimization Results

Once optimization completes, QuickQuan creates a tune report that includes tune status, breakdown curves, and MS/MS spectra. View the optimization results using any of the following procedures:

- "Viewing Results in the Optimization Tune Report View" on page 36
- "Generating an Optimization Summary Report in Excel" on page 39
- "Using Adobe Acrobat Reader to View the Results" on page 39

Tip Compounds that do not tune correctly appear in red and the status is NOT TUNED.

Viewing Results in the Optimization Tune Report View

You can view the tune report in the Optimization Tune Report view. The tune reports for each compound are also stored as PDF files in the PDF/RAW Output Path folder that you specified in the Optimization Setup view. (See "Specifying Tune and Method Files and Optimization Settings" on page 25.) You can also open the Xcalibur Qual Browser to see the display of raw data results for the selected compound.

❖ To display the Optimization Tune Report view

In the QuickQuan navigation pane, click **Optimization**, and then click **Tune Report**.

❖ To view a tune report

1. In the Optimization Tune Report view, select the compound from the list on the left side. See Figure 25 and Figure 26. QuickQuan automatically displays the latest tune report for the compound.
2. To display the raw sample data collected for the compound, click **QualBrowser**. Xcalibur Qual Browser opens and displays the raw data.

Figure 25. Optimization Tune Report view, page 1

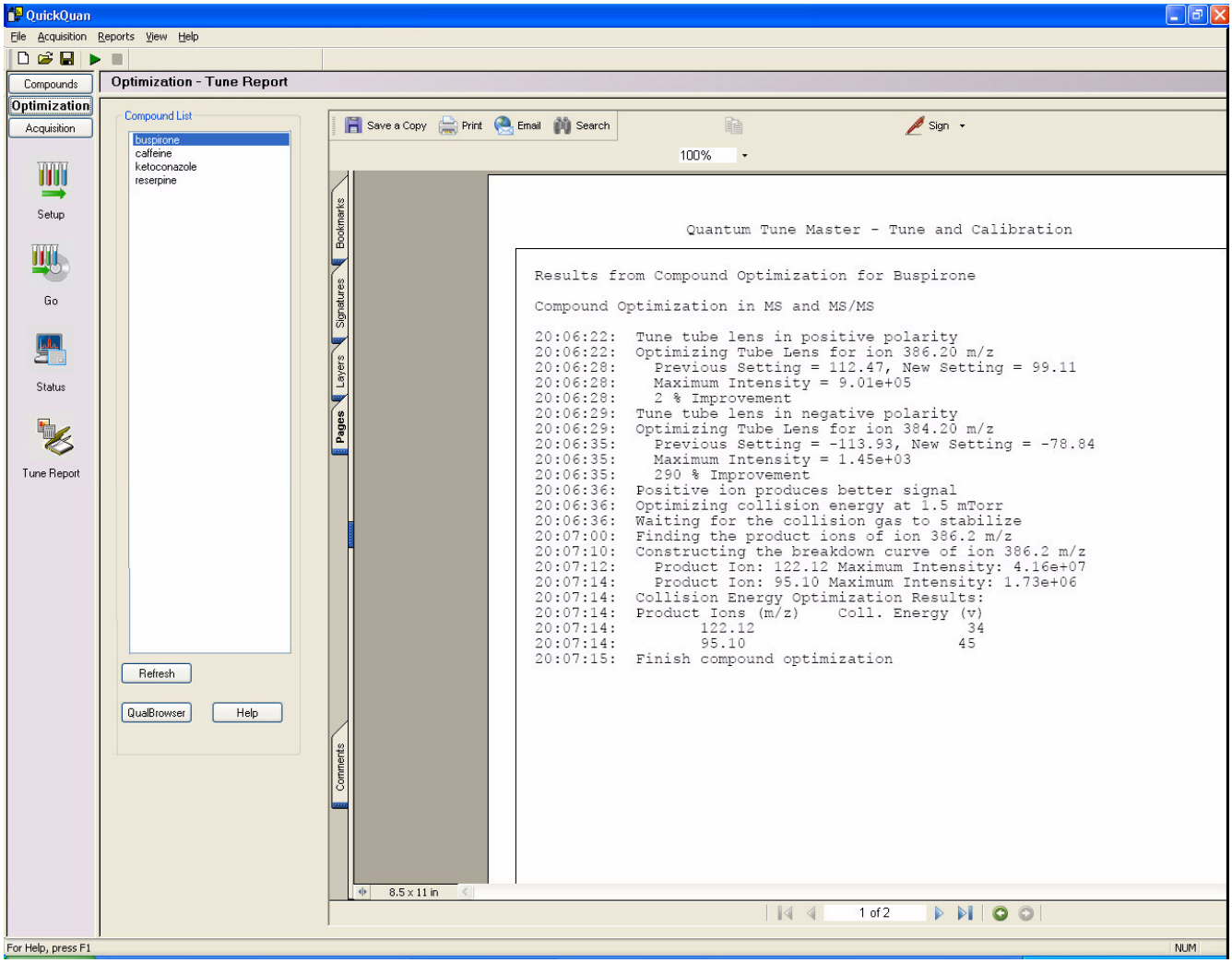
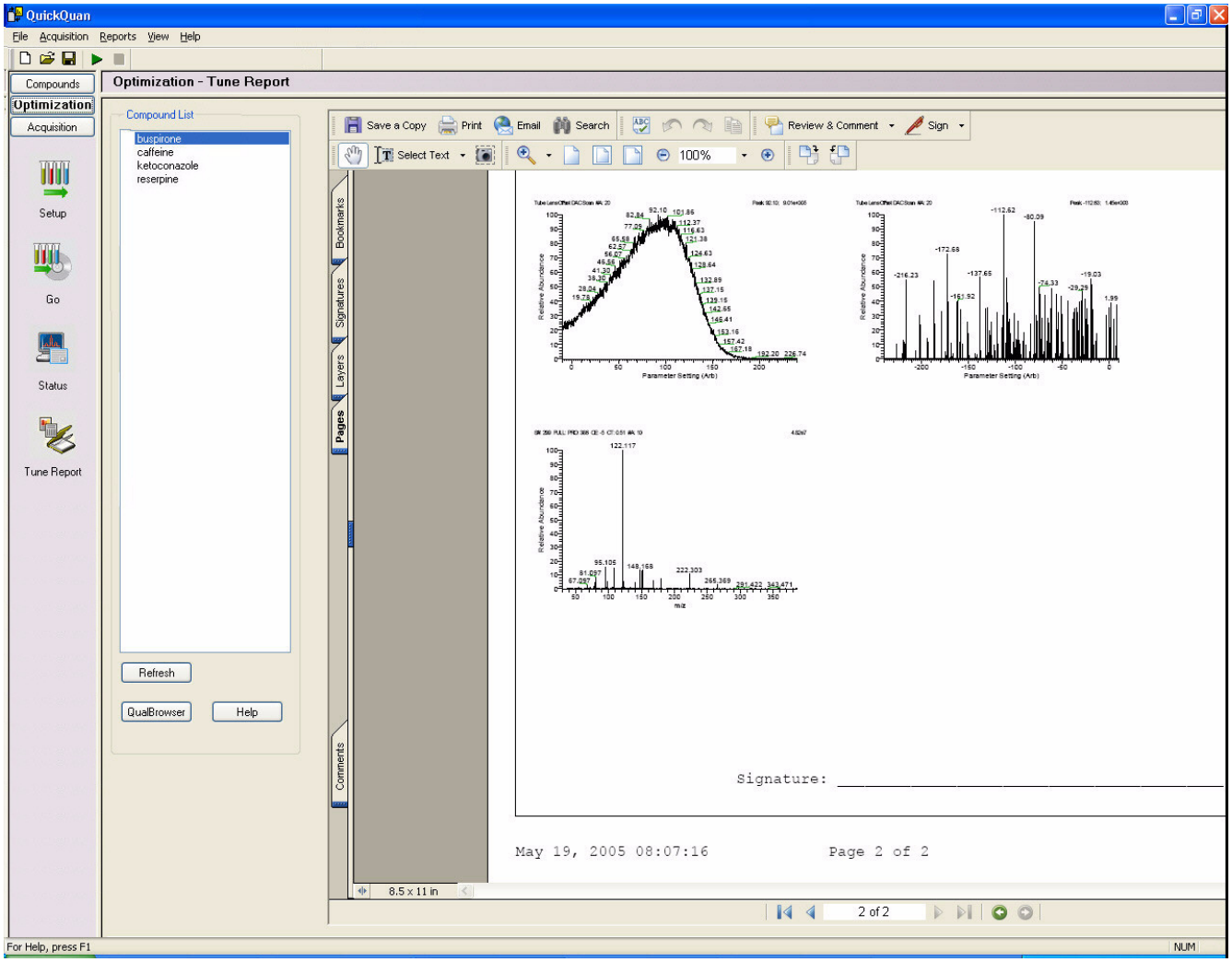


Figure 26. Optimization Tune Report view, page 2



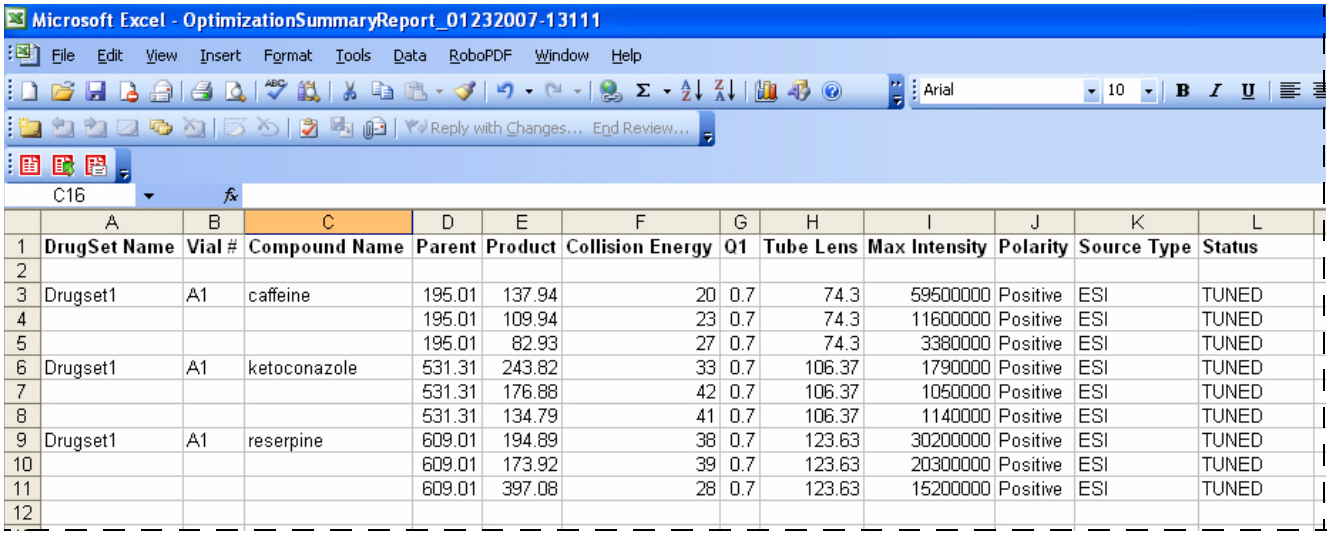
Generating an Optimization Summary Report in Excel

❖ **To generate the optimization summary report in an Excel spreadsheet**

In the QuickQuan window, choose **Reports > Optimization Summary Report**.

Figure 27 shows an example of an optimization summary report for a tune plate.

Figure 27. Optimization summary report


Microsoft Excel - OptimizationSummaryReport_01232007-13111
File Edit View Insert Format Tools Data RoboPDF Window Help
Arial 10
Reply with Changes... End Review...
C16

	A	B	C	D	E	F	G	H	I	J	K	L
1	DrugSet Name	Vial #	Compound Name	Parent	Product	Collision Energy	Q1	Tube Lens	Max Intensity	Polarity	Source Type	Status
2												
3	Drugset1	A1	caffeine	195.01	137.94	20	0.7	74.3	59500000	Positive	ESI	TUNED
4				195.01	109.94	23	0.7	74.3	11600000	Positive	ESI	TUNED
5				195.01	82.93	27	0.7	74.3	3380000	Positive	ESI	TUNED
6	Drugset1	A1	ketoconazole	531.31	243.82	33	0.7	106.37	1790000	Positive	ESI	TUNED
7				531.31	176.88	42	0.7	106.37	1050000	Positive	ESI	TUNED
8				531.31	134.79	41	0.7	106.37	1140000	Positive	ESI	TUNED
9	Drugset1	A1	reserpine	609.01	194.89	38	0.7	123.63	30200000	Positive	ESI	TUNED
10				609.01	173.92	39	0.7	123.63	20300000	Positive	ESI	TUNED
11				609.01	397.08	28	0.7	123.63	15200000	Positive	ESI	TUNED
12												

Using Adobe Acrobat Reader to View the Results

The Adobe® Acrobat Reader® software can be installed from the QuickQuan software CD.

❖ **To view the tune results report using Adobe Acrobat Reader**

1. Start Adobe Acrobat Reader.
2. Open the PDF files for the tune results, for example, caffeine.pdf.

Updating SRM Information

You can update the SRM transitions that QuickQuan found during optimization. See one of the following procedures:

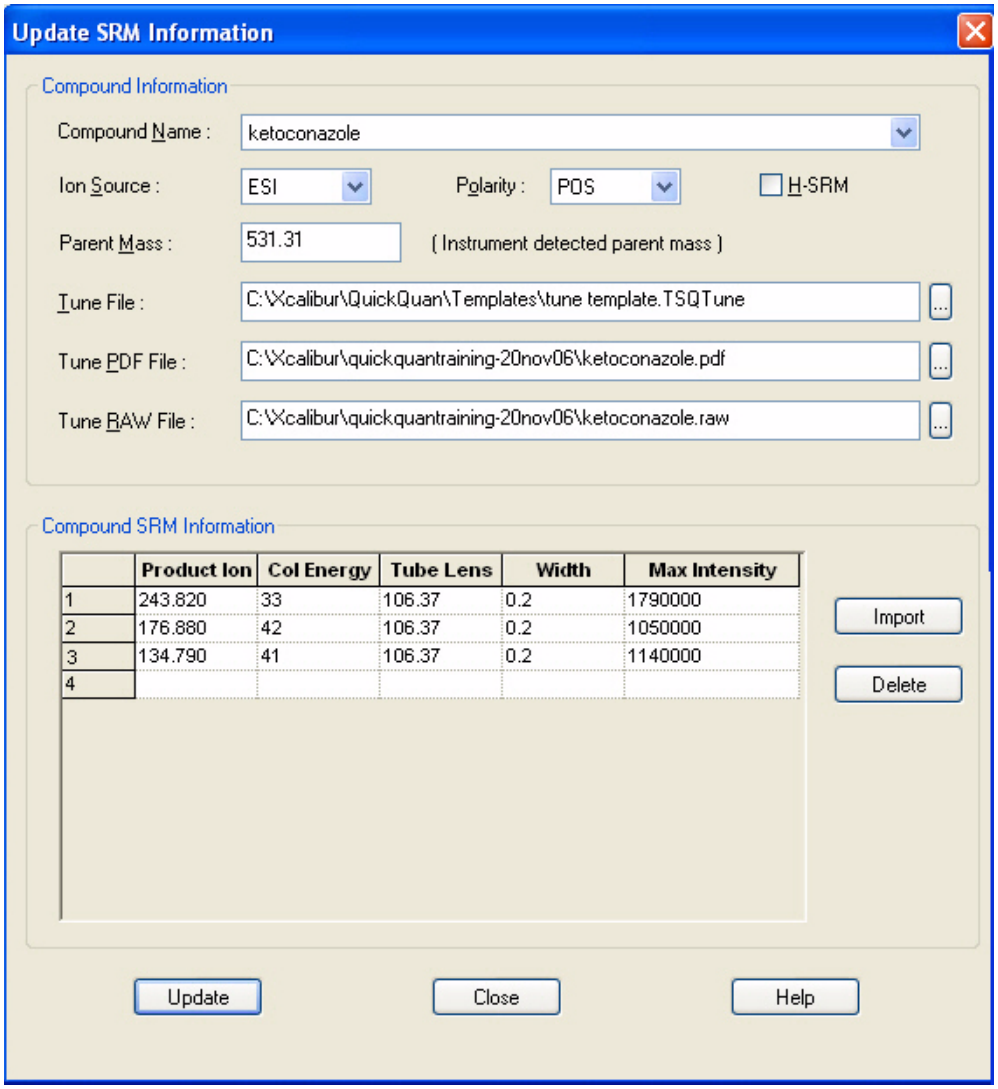
- "Modifying SRM Information Manually" on page 40
- "Importing SRM Information" on page 41

Modifying SRM Information Manually

❖ To modify SRM information

1. In the QuickQuan navigation pane, click **Compounds**.
2. In the Compounds Browse view, click **Update SRM Info**. The Update SRM Information dialog box appears. See Figure 28.

Figure 28. Update SRM Information dialog box



3. In the Compound Name box, select a compound.
4. In the Compound SRM Information table, edit the information as required.
5. Click **Update** to update the SRM information.
6. Click **Close**.

Importing SRM Information

You can import the SRM information from a text file (.txt) into a QuickQuan database. The text file must be in a specified format. QuickQuan includes an example text file in the following folder:

\Xcalibur\QuickQuan\ImportFiles

❖ To create an SRM information file for importing

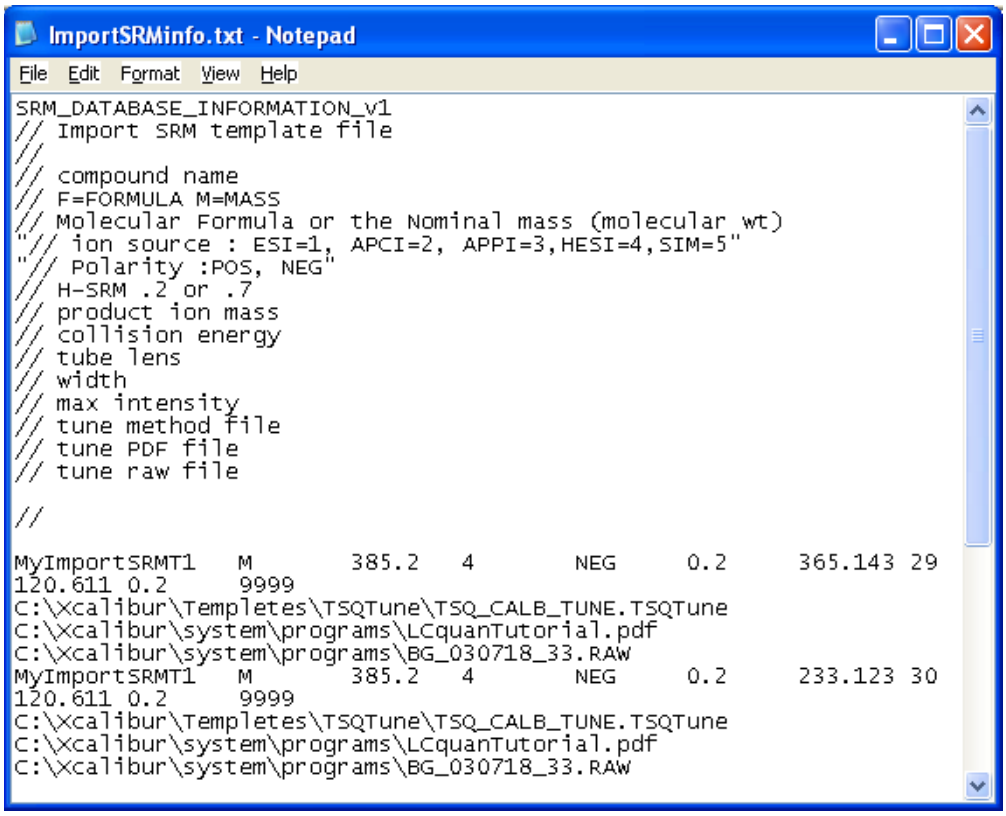
1. Open a file in Microsoft Excel, Notepad, or any of the software that allows you to create a tab-delimited text file (.txt file extension).
2. Enter the following string in the first row of a text file:

   SRM_DATABASE_INFORMATION_v1
3. (Optional) To include a comment in the file, use a double forward slash (//) at the start of the row. The software ignores any rows that begin with //.
4. In each row, enter the following information. Use a tab to separate each entry in the row.

   compound name
   F= formula or M= mass
   molecular formula or nominal mass (molecular wt)
   ion source: ESI=1, APCI=2, APPI=3, HESI=4, or SIM=5
   polarity: POS or NEG
   H-SRM .2 or .7
   product ion mass
   collision energy
   tube lens
   width
   maximum intensity
   tune method file
   tune PDF file
   tune raw file

   Figure 29 shows an example text file.
5. Save the file as a .txt file.

Figure 29. Example of File for Importing SRM Information



❖ To import the SRM information file

1. In the QuickQuan navigation pane, click **Compounds**.
2. In the Compounds Browse view, click **Update SRM Info**. The Update SRM Information dialog box appears.
3. Click **Import**.
4. Click **Yes** when the confirmation message appears.
5. In the Open dialog box, select the file you want to import, and then click **Open**. QuickQuan imports the compounds and SRM transitions into the database.
6. Click **Update**, and then click **Close**.

Acquiring the Sample Data

This chapter describes how to set up and run a high-throughput acquisition using QuickQuan.

Contents

- Reusing Acquisition Settings
- Creating a Generic Instrument Method
- Creating a Generic Processing Method
- Specifying Template Options
- Creating or Importing a Sequence
- Importing Excel and Sequence Templates
- Saving the QuickQuan Assay
- Running an Acquisition
- Stopping an Acquisition
- Exporting the Instrument and Processing Methods

Reusing Acquisition Settings

You can reuse the settings from an acquisition (.aql file) that you have already created in QuickQuan. The .aql file contains the configuration settings, acquisition settings, compound optimization information, assay layout, and template information.

❖ To reuse the settings in an .aql file

1. In the QuickQuan window, choose **File > Open**.
2. In the Open dialog box, select the .aql file, and then click **Open**. For an example, open the following:

   \Xcalibur\examples\QuickQuan\SampleSet\acquire template.aql

3. In the QuickQuan navigation pane, click **Acquisition**. Verify the acquisition settings in the following views:

Click **Templates** to view the settings in the Acquisition Templates view. To edit the template settings, see "Specifying Template Options" on page 53.

Click **Setup** to view the sequence settings in the Acquisition Setup view. To edit the sequence settings, see "Creating or Importing a Sequence" on page 55.

Creating a Generic Instrument Method

You specify certain settings for the mass spectrometer, autosampler, and LC pump in a generic instrument method (.meth file), which you create in Xcalibur Instrument Setup. QuickQuan uses the generic instrument method and the optimized settings that it determines during compound optimization to build the complete instrument method for the assay.

QuickQuan alters the masses and mass ranges specified in the scan event of the generic instrument method based on the information retrieved from the database for each compound. QuickQuan makes the following adjustments to the instrument method file for the mass spectrometer:

- Creates the parent-product transition pairs from the information it retrieves from the database for each compound.
- Uses this information to create and replicate, as necessary, scan events for the internal standard, if specified, and for all compounds used within the drug set for this sequence.
- Adds all SRM transitions for each compound to the SRM table of the scan event for the compound.

QuickQuan does not alter instrument methods for the autosampler, LC pump, or other detectors.

Note You can specify different LC methods for different samples within a sequence,. For example, you might use multiple pumps within the same sequence. See "Bypassing the LC Column and the Dual-Pump, Dual-Column Configuration" on page 81.

❖ To create a generic instrument method

1. Start Xcalibur Instrument Setup as follows:
   a. In the QuickQuan navigation pane, click **Acquisition**, and then click **Templates**.
   b. In the Acquisition Templates view, click **Inst Setup**. The Xcalibur Instrument Setup view appears. Figure 30 shows the Instrument Setup view.
2. (Optional) To use an example file as the basis for a new instrument method, choose **File > Open**, and then select a .meth file from the following folder:

   \Xcalibur\QuickQuan\Templates

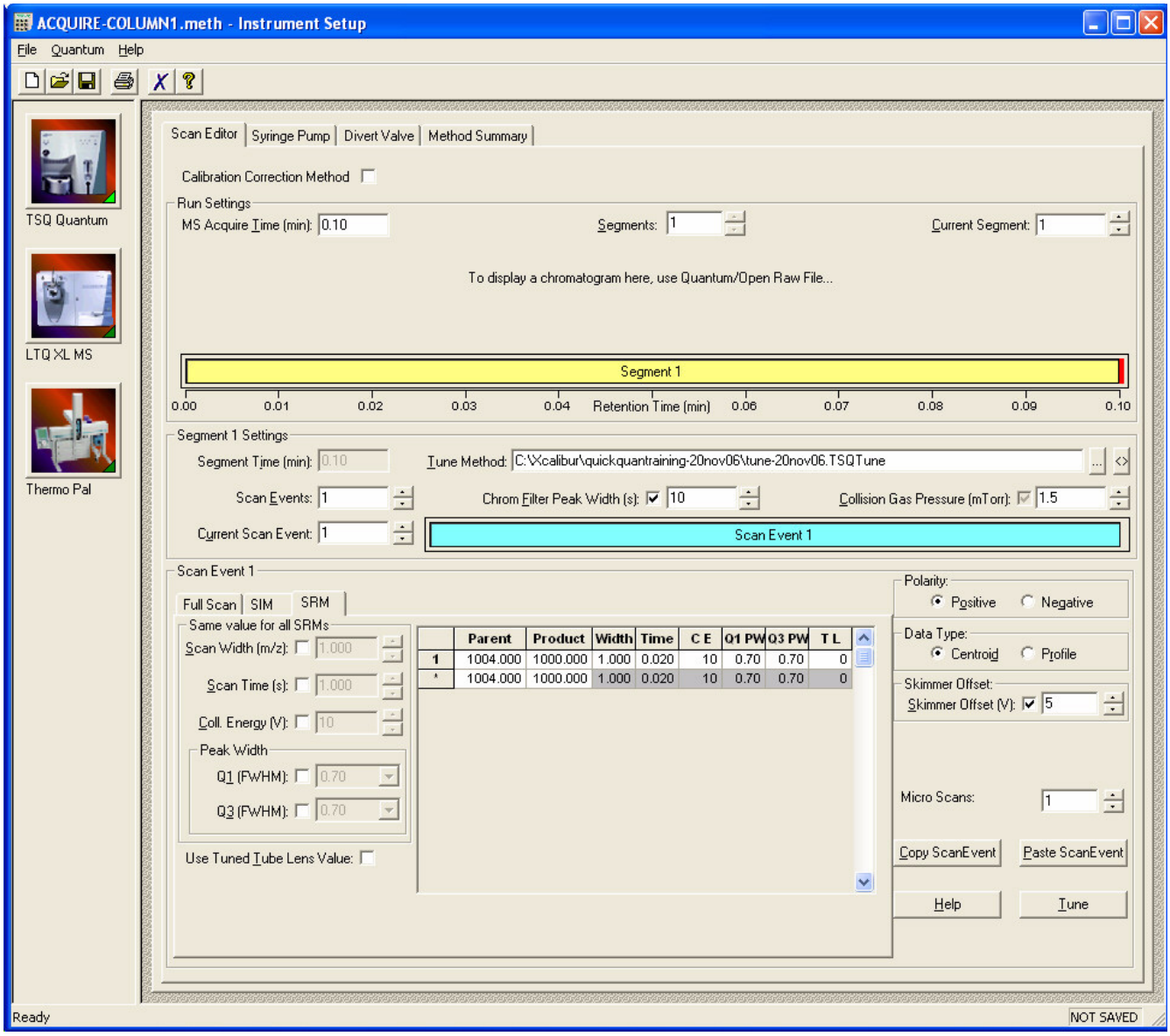
3. Verify the following mass spectrometer settings:
   - Segments: 1
   - Scan Events: 1
   - Scan Type: SRM

   QuickQuan uses the scan type to determine how the compounds will be scanned.
4. Enter the following mass spectrometer settings:
   - MS acquire time (min)
   - Tune method (not optimized)

     See the following example method:

     \Xcalibur\examples\QuickQuan\SampleSet\ tune template.TSQTune
5. Click the **Divert Valve** tab, and then enter the divert valve settings on the Divert Valve page.
6. Choose **File > Save As**. Type a new file name (.meth file extension) and then click **Save**.

Figure 30. Instrument Setup view



Creating a Generic Processing Method

A processing method is a defined set of parameters that provide Xcalibur and QuickQuan with a recipe for automatic quantitation. You use Xcalibur Processing Setup to create a generic processing method (.pmd file) for automated batch analysis. QuickQuan uses the generic processing method as the base for creating a processing method for each drug set in each sequence in the assay.

QuickQuan modifies the generic method based on the component information and the data acquired. To create the initial processing method, QuickQuan does the following.

- The generic ISTD component, if specified, is renamed using the ISTD compound names you selected. A partial scan filter is created to match the instrument method scan filter for each ISTD component. QuickQuan retrieves the information for each ISTD from the database and inserts it in the instrument method.
- The generic target component is modified in the same manner as the generic ISTD component. The mass range is set to be the product mass range and the scan filter is set to SRM.

After the acquisition, the software does further refining of the processing method.

The generic processing method requires the following:

- Components: An external standard method must specify only one component, which is named *target*. An internal standard (ISTD) method must specify two components, which are named *target* and *istd.*
- Calibration level and QC names and amounts
- Calibration curve settings
- Detection settings

❖ To create a generic processing method

1. Start Xcalibur Processing Setup:
   a. Display the Acquisition Templates view:

      In the QuickQuan navigation pane, click **Acquisition**, and then click the **Templates** button.

   b. On the Acquisition Templates view, click **Proc Setup**. The Xcalibur Processing Setup view appears. Figure 31 shows the Processing Setup view.

2. (Optional) To use an example file as the basis for your processing method, choose **File > Open**, and then select a .pmd file. QuickQuan includes the following examples:

   \Xcalibur\QuickQuan\Templates\Thermo_template_ExtStd.pmd
   (method for external standards)

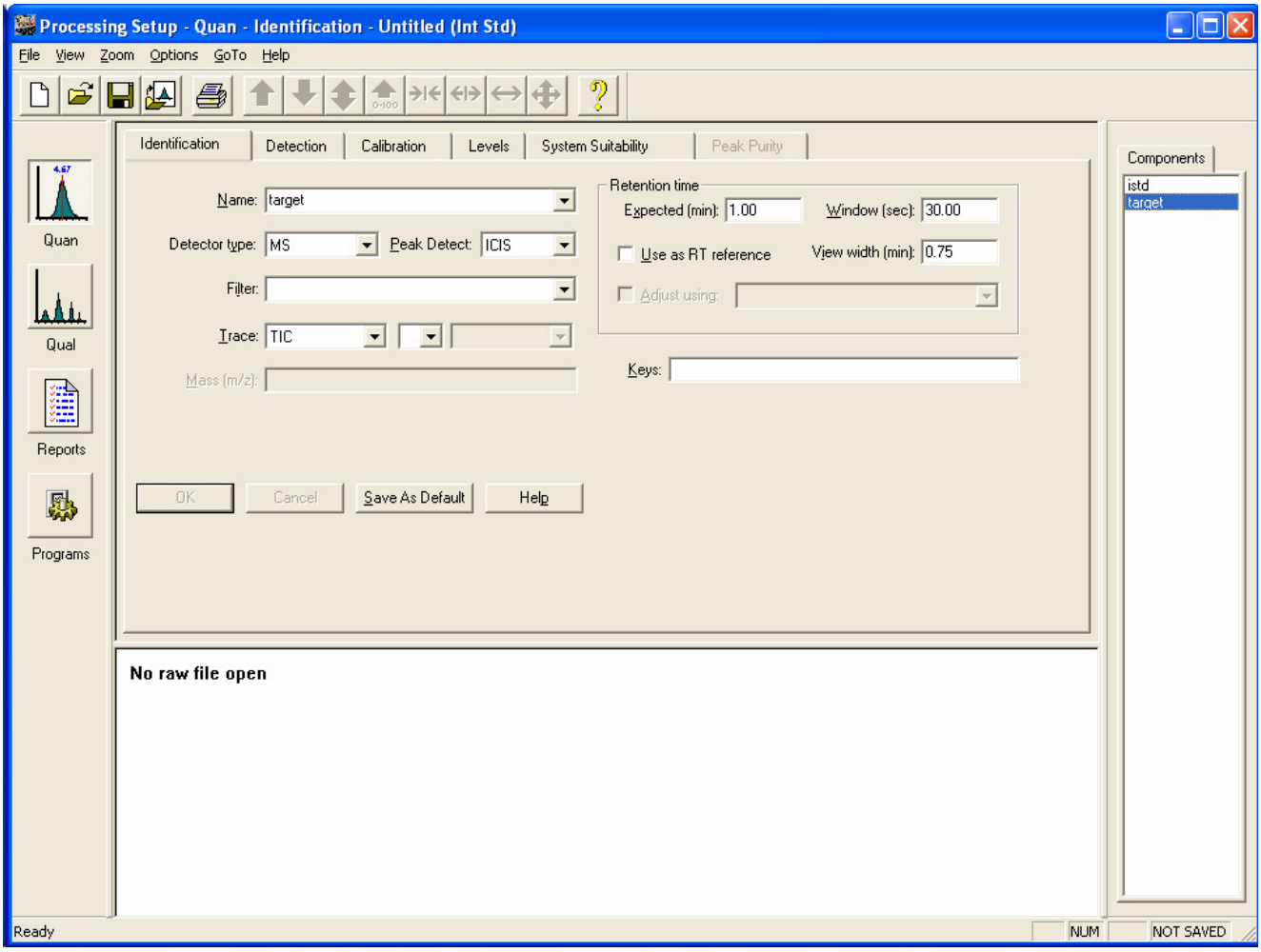
   \Xcalibur\QuickQuan\Templates\Thermo_template_IntStd.pmd
   (method for internal standards)

   If you use one of these examples, go to step 5 to edit the example.

3. On the Identification page, create a component named *target* as follows:
   a. In the Name list, select **New**.
   b. Type **target** using lowercase letters.
   c. Click **OK**. The target component appears in the Components list.

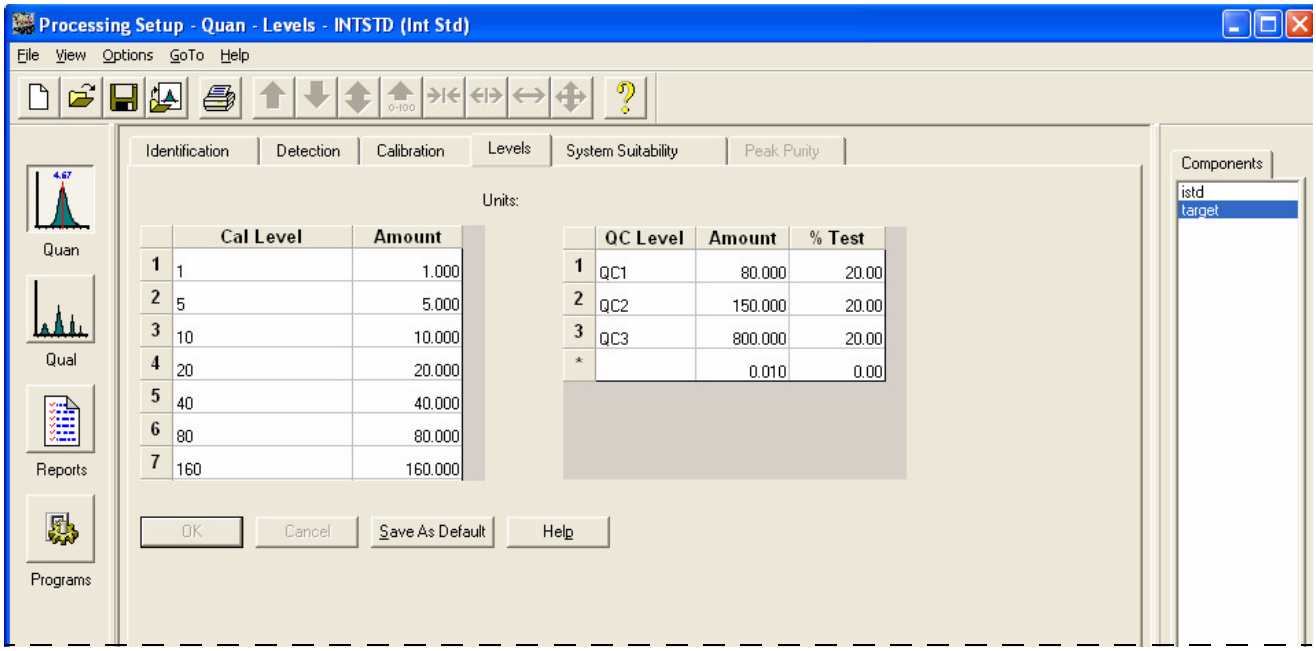
4. (ISTD only) Create a component named *istd* as follows:
   a. In the Name list, select **New**.
   b. Type **istd** using lowercase letters.
   c. Click **OK**. The istd component appears in the Components list.

Figure 31. Processing Setup – Quan view – Identification page



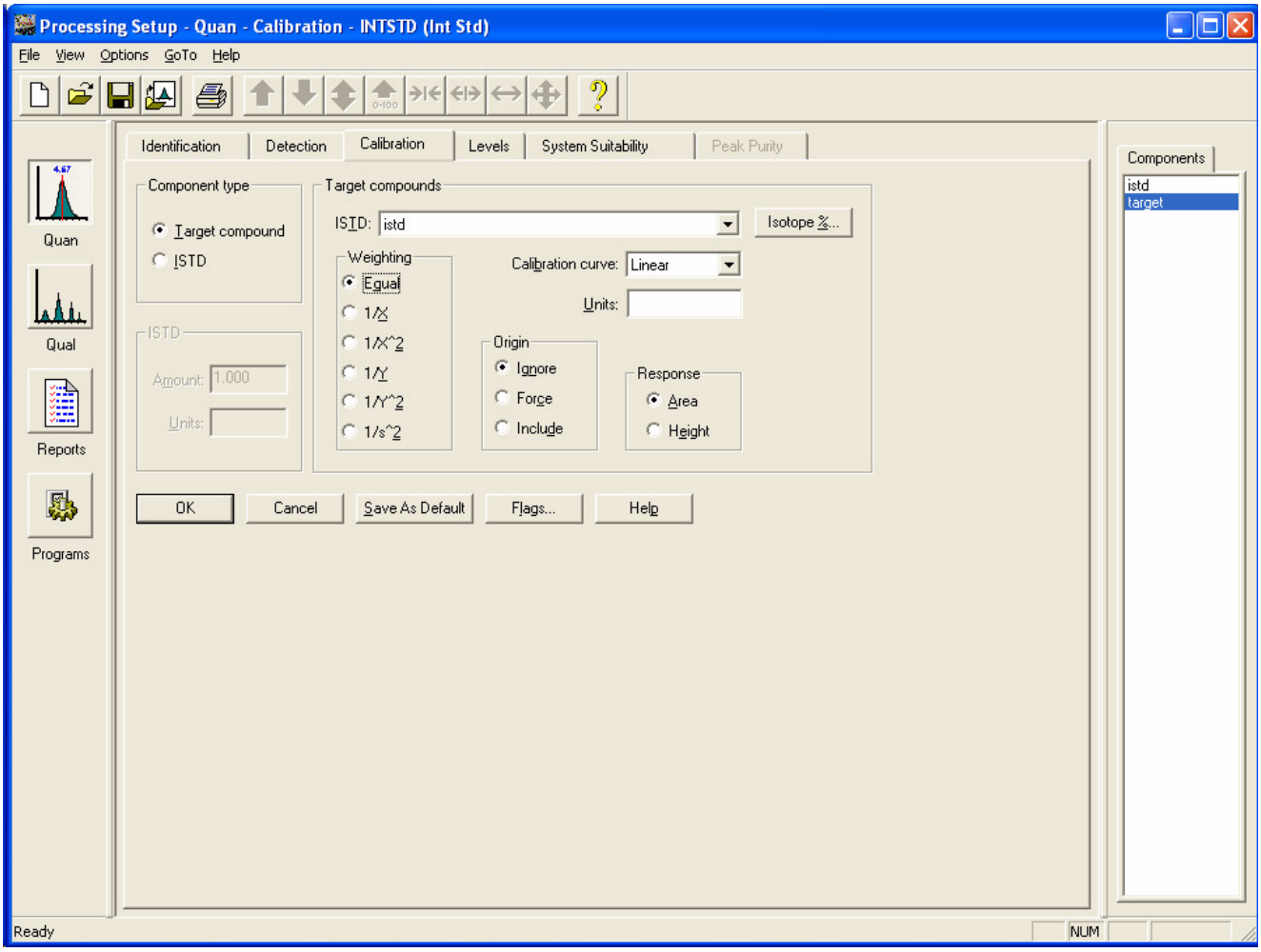
5. On the Levels page, enter the calibration levels:
   a. In the components list, select **target**.
   b. Enter the calibration and QC level names and amounts for your standards (external or internal) and QCs.
   c. Click **OK**. Figure 32 shows an example.

Figure 32. Processing Setup – Quan view – Levels page



6. (ISTD only) On the Calibration page, specify that *istd* is the internal standard as follows:
   a. In the Components list, select **istd**.
   b. In the Component type area, select **ISTD**.
   c. Click **OK**.
7. On the Calibration page, specify that *target* is the target compound as follows:
   a. In the Components list, select **target**.
   b. In the Component type area, select **Target compound**.
   c. (ISTD only) In the Target compounds ISTD list, select **istd**.
   d. Click **OK**.
8. On the Calibration page, enter the settings for the calibration curve, and then click **OK**. See Figure 33 for an example.

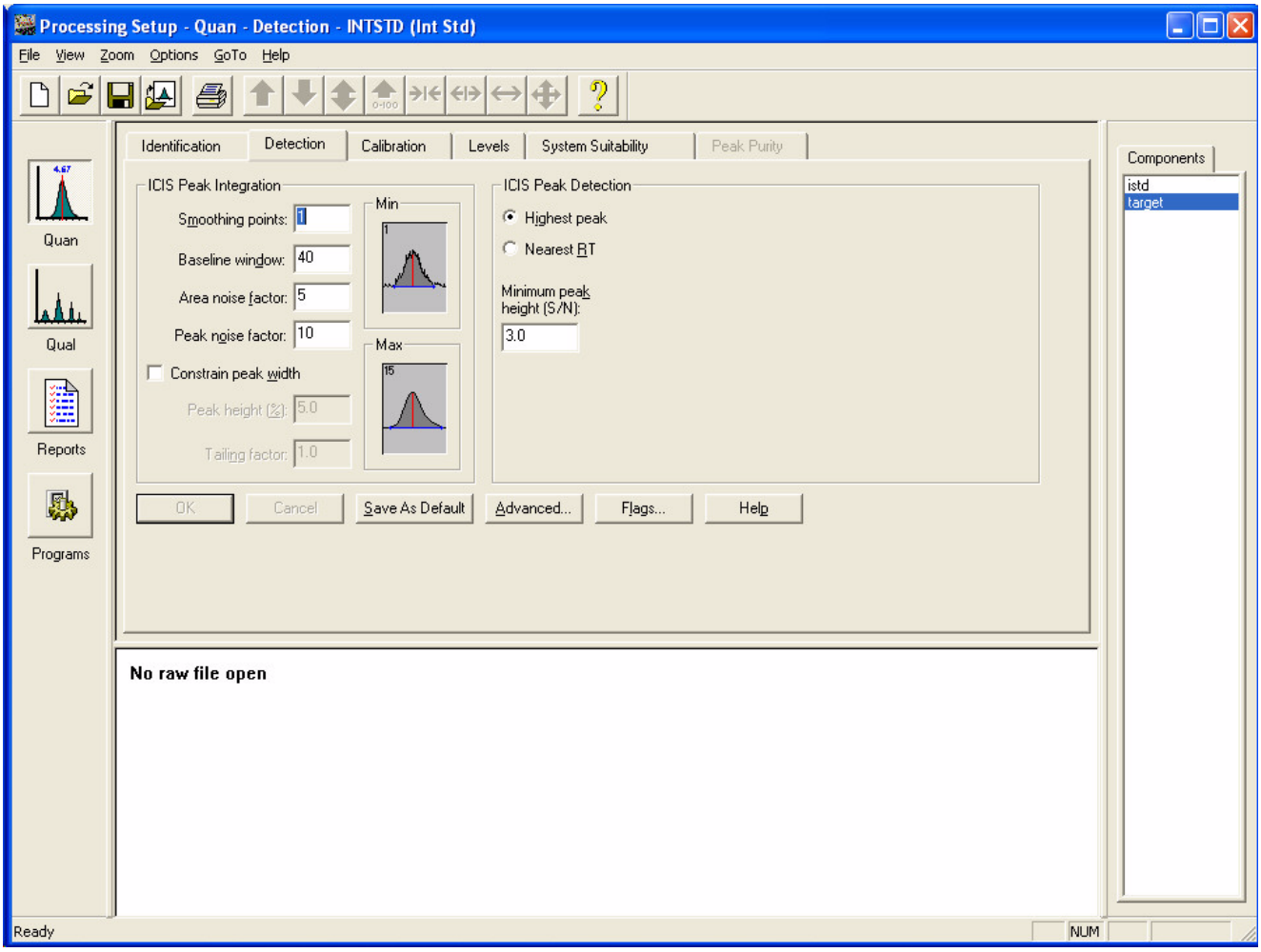
Figure 33. Processing Setup – Quan view – Calibration page



9. On the Detection page (Figure 34), enter the detection settings. For more details, click **Help**.

10. Choose **File > Save As**. Type a new file name (.pmd file extension) and then click **Save**.

Figure 34. Processing Setup – Quan view – Detection page



Specifying Template Options

The template options include the location of the generic instrument and processing methods, which internal standards (ISTDs) to use, and the output folder. You specify the template options in the Acquisition Templates view.

❖ To open Acquisition Templates view

In the QuickQuan navigation pane, click **Acquisition**, and then click **Templates**. See Figure 35.

❖ To specify template options

1. In the Generic Instrument Method box, click ..., and then select the method (.meth file) you created in "Creating a Generic Instrument Method" on page 44.
2. In the Generic Processing Method box, click ..., and then select the method (.pmd file) you created in "Creating a Generic Processing Method" on page 47.
3. (Optional) In the Processing Macro Template box, specify a macro to perform custom manipulations of the data acquisition results. To do this, click ..., and then select the Excel template file (.xls) that was designed to invoke that macro automatically.

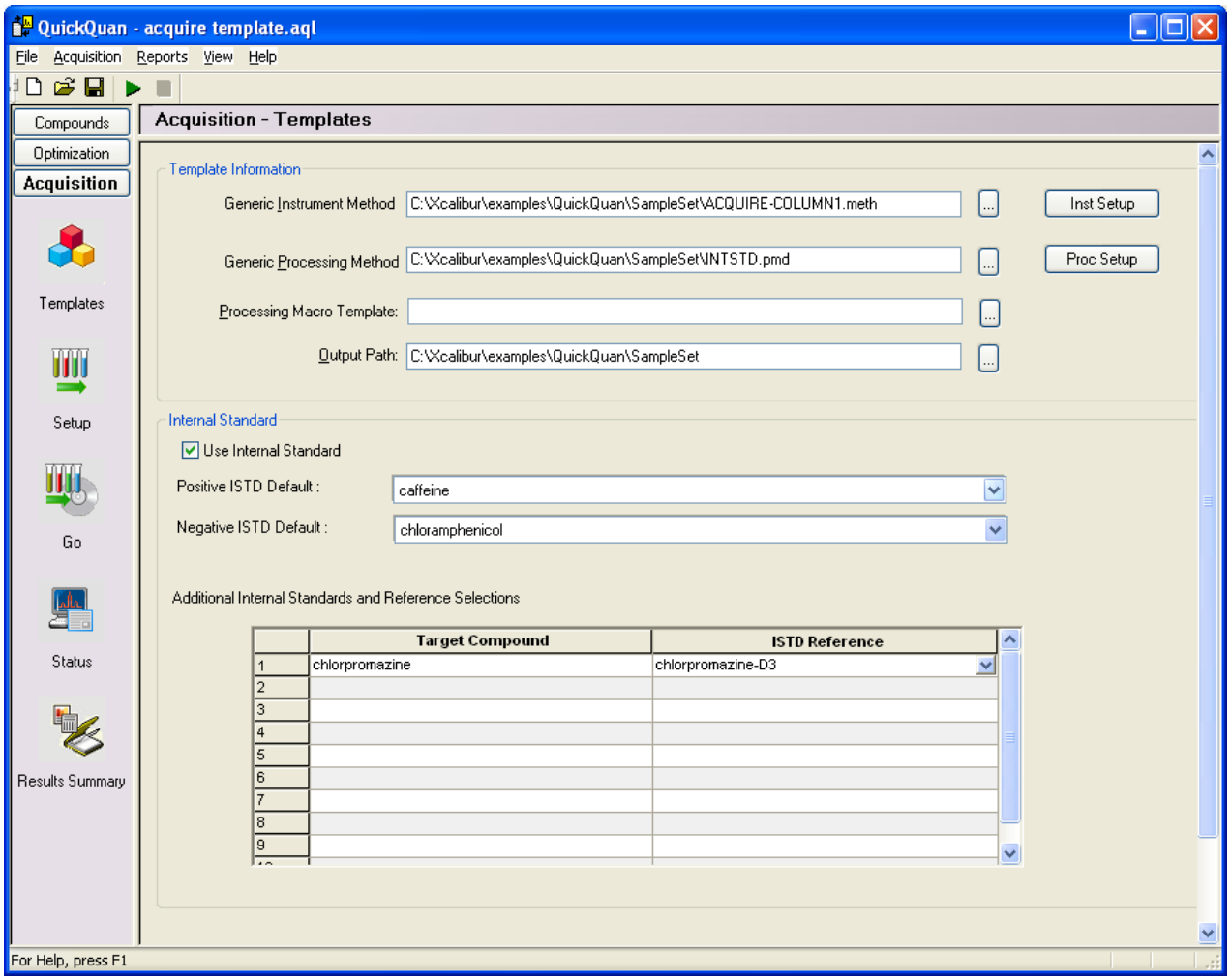
   For more information, see "Using a Macro To Perform Custom Calculations" on page 83.
4. In the Output Path box, click ..., and then select the folder where you want QuickQuan to create a time-and-date-stamped folder to store the data and method files for the acquisition (for example, files with the file extensions .raw, .meth, .pmd, .sld, and .pdf).

   Note The sample data (.raw) and the PDF files are stored in the QuickQuan database. The .raw files can be read using any Xcalibur software that supports .raw data files. Adobe Acrobat Reader is required to view the PDF files.
5. (Optional) Select the positive and negative internal standards from the QuickQuan database as follows:
   a. Select the **Use Internal Standard** check box.
   b. In the Positive ISTD Default and Negative ISTD Default lists, select the compounds you want QuickQuan to use by default.
   c. (Optional) In the Target Compound and ISTD Reference table, specify any additional compounds to override the defaults specified in step b. Click the table cell to display the list of compounds.

QuickQuan includes the default ISTD compounds as separate components in each new processing method. The positive compounds reference the default positive ISTD, and the negative compounds reference the default negative ISTD, unless you specify additional ISTDs in the table. Each ISTD in the table is also included in the processing method and references the target compound specified in the table.

Figure 35 shows the Acquisition Templates view that uses the processing method and instrument method that were created earlier.

Figure 35. Acquisition Templates view



Creating or Importing a Sequence

The Acquisition Setup view allows you to set up a sequential sequence containing unknown samples, calibration standard samples, quality control samples, and blank samples. One row of the sequence corresponds to one sample injection. Each injection is defined by the settings in its sequence row. The number of calibration levels in each calibration set is defined by the processing method that you created in "Creating a Generic Processing Method" on page 47.

To create a sequence, use one of the following procedures:

- "Creating a Sequence in the Acquisition Setup View" on page 55
- "Copying Sequences from Excel" on page 57
- "Importing a Sequence" on page 58
- "Importing Excel and Sequence Templates" on page 59

Creating a Sequence in the Acquisition Setup View

In the Acquisition Setup view, you can create multiple sequences for an assay.

❖ To display the Acquisition Setup view

In the QuickQuan navigation pane, click **Acquisition**, and then click **Setup**.

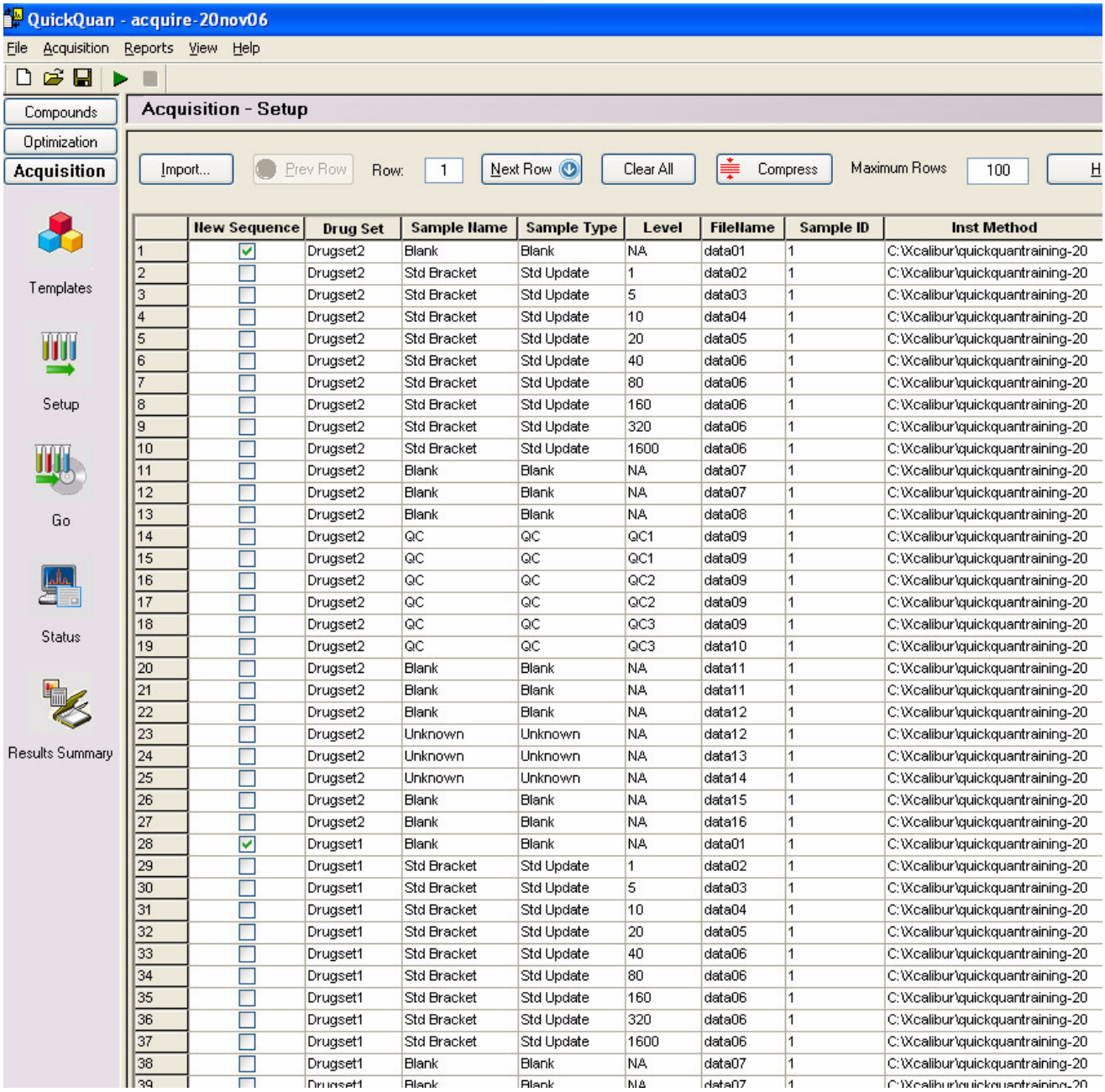
❖ To create sequences in the Acquisition Setup view

1. In the sequence grid, select the **New Sequence** check box to designate the start of a new sequence. See Figure 36.
2. Enter the sample information in each row of the sequence. For a description of each column in the sequence grid, see "Acquisition Setup View" on page 99.

   You can repeat these steps to add additional sequences.
3. Choose **File > Save** to save the sequences to the assay (.aql file).

For a description of ways to edit the sequence grid, see "Editing a Sequence in the Acquisition Setup View" on page 57.

Figure 36. Acquisition Setup view, showing the sequences for Drugset1 and Drugset2



	New Sequence	Drug Set	Sample Name	Sample Type	Level	FileName	Sample ID	Inst Method
1	☑	Drugset2	Blank	Blank	NA	data01	1	C:\Xcalibur\quickquantraining-20
2	☐	Drugset2	Std Bracket	Std Update	1	data02	1	C:\Xcalibur\quickquantraining-20
3	☐	Drugset2	Std Bracket	Std Update	5	data03	1	C:\Xcalibur\quickquantraining-20
4	☐	Drugset2	Std Bracket	Std Update	10	data04	1	C:\Xcalibur\quickquantraining-20
5	☐	Drugset2	Std Bracket	Std Update	20	data05	1	C:\Xcalibur\quickquantraining-20
6	☐	Drugset2	Std Bracket	Std Update	40	data06	1	C:\Xcalibur\quickquantraining-20
7	☐	Drugset2	Std Bracket	Std Update	80	data06	1	C:\Xcalibur\quickquantraining-20
8	☐	Drugset2	Std Bracket	Std Update	160	data06	1	C:\Xcalibur\quickquantraining-20
9	☐	Drugset2	Std Bracket	Std Update	320	data06	1	C:\Xcalibur\quickquantraining-20
10	☐	Drugset2	Std Bracket	Std Update	1600	data06	1	C:\Xcalibur\quickquantraining-20
11	☐	Drugset2	Blank	Blank	NA	data07	1	C:\Xcalibur\quickquantraining-20
12	☐	Drugset2	Blank	Blank	NA	data07	1	C:\Xcalibur\quickquantraining-20
13	☐	Drugset2	Blank	Blank	NA	data08	1	C:\Xcalibur\quickquantraining-20
14	☐	Drugset2	QC	QC	QC1	data09	1	C:\Xcalibur\quickquantraining-20
15	☐	Drugset2	QC	QC	QC1	data09	1	C:\Xcalibur\quickquantraining-20
16	☐	Drugset2	QC	QC	QC2	data09	1	C:\Xcalibur\quickquantraining-20
17	☐	Drugset2	QC	QC	QC2	data09	1	C:\Xcalibur\quickquantraining-20
18	☐	Drugset2	QC	QC	QC3	data09	1	C:\Xcalibur\quickquantraining-20
19	☐	Drugset2	QC	QC	QC3	data10	1	C:\Xcalibur\quickquantraining-20
20	☐	Drugset2	Blank	Blank	NA	data11	1	C:\Xcalibur\quickquantraining-20
21	☐	Drugset2	Blank	Blank	NA	data11	1	C:\Xcalibur\quickquantraining-20
22	☐	Drugset2	Blank	Blank	NA	data12	1	C:\Xcalibur\quickquantraining-20
23	☐	Drugset2	Unknown	Unknown	NA	data12	1	C:\Xcalibur\quickquantraining-20
24	☐	Drugset2	Unknown	Unknown	NA	data13	1	C:\Xcalibur\quickquantraining-20
25	☐	Drugset2	Unknown	Unknown	NA	data14	1	C:\Xcalibur\quickquantraining-20
26	☐	Drugset2	Blank	Blank	NA	data15	1	C:\Xcalibur\quickquantraining-20
27	☐	Drugset2	Blank	Blank	NA	data16	1	C:\Xcalibur\quickquantraining-20
28	☑	Drugset1	Blank	Blank	NA	data01	1	C:\Xcalibur\quickquantraining-20
29	☐	Drugset1	Std Bracket	Std Update	1	data02	1	C:\Xcalibur\quickquantraining-20
30	☐	Drugset1	Std Bracket	Std Update	5	data03	1	C:\Xcalibur\quickquantraining-20
31	☐	Drugset1	Std Bracket	Std Update	10	data04	1	C:\Xcalibur\quickquantraining-20
32	☐	Drugset1	Std Bracket	Std Update	20	data05	1	C:\Xcalibur\quickquantraining-20
33	☐	Drugset1	Std Bracket	Std Update	40	data06	1	C:\Xcalibur\quickquantraining-20
34	☐	Drugset1	Std Bracket	Std Update	80	data06	1	C:\Xcalibur\quickquantraining-20
35	☐	Drugset1	Std Bracket	Std Update	160	data06	1	C:\Xcalibur\quickquantraining-20
36	☐	Drugset1	Std Bracket	Std Update	320	data06	1	C:\Xcalibur\quickquantraining-20
37	☐	Drugset1	Std Bracket	Std Update	1600	data06	1	C:\Xcalibur\quickquantraining-20
38	☐	Drugset1	Blank	Blank	NA	data07	1	C:\Xcalibur\quickquantraining-20
39	☐	Drugset1	Blank	Blank	NA	data07	1	C:\Xcalibur\quickquantraining-20

Editing a Sequence in the Acquisition Setup View

You can edit the sequence in the Acquisition Setup view. For a description of each column in the sequence grid, see "Acquisition Setup View" on page 99.

❖ To fill down the entries from one row to a contiguous range of rows

1. Click the row that you want to copy, right-click the table, and then choose **Fill Down** from the shortcut menu.
2. In the Fill Down dialog box, select the columns to be duplicated, select the destination rows, and then click **OK**.

❖ To insert a row in the sequence grid

Right-click the row below the target location, and then choose **Insert Rows** from the shortcut menu.

❖ To delete a row from the sequence grid

Click the row number to highlight the entire row, right-click the selection, and then choose **Delete Rows**.

Copying Sequences from Excel

You can copy sequences or portions of a sequence from a Microsoft Excel file to the Acquisition Setup view. You can also copy sequences from the Acquisition Setup view to an Excel file. The copied sequence can contain all the columns that appear in the Acquisition Setup view, including the drug set name.

❖ To copy sequences from an Excel file to QuickQuan

1. In the Excel file, verify that the column headings and column order match the columns in the Acquisition Setup view.
2. Select the columns and rows of the sequence in the Excel file, and then press CTRL+C.
3. In the Acquisition Setup view, position the pointer in the sequence grid, and then press CTRL+V.
4. Verify that the correct values appear.

❖ To copy sequences from the Acquisition Setup view to an Excel file

1. In the Acquisition Setup view, select the columns and rows that you want to copy, and then press CTRL+C.
2. In the Excel file, position the pointer in the grid and then press CTRL+V.

Tip You can also copy portions of the sequence grid from the Acquisition Setup view and paste the copy into an Excel file. To do this, highlight the columns and rows in the Acquisition Setup view, and then press CTRL+C. In the Excel file, position the pointer in the grid, and then press CTRL+V.

Importing a Sequence

You can import a sequence (.sld, .txt, or .csv file) that you created previously in Xcalibur Sequence Setup. See "Acquisition Setup View" on page 99 for a description of the sequence columns. You can import the information for all the columns in the QuickQuan sequence grid, except the New Sequence and Drug Set columns.

Tip Instead of importing a sequence, you can copy the sequence from a Microsoft Excel file to the Acquisition Setup view. The copy can contain all columns that appear in the Acquisition Setup view, including the Drug Set column. See "Copying Sequences from Excel" on page 57.

❖ To display the Acquisition Setup view

In the QuickQuan navigation pane, click **Acquisition**, and then click **Setup**.

❖ To import a sequence

1. In the Acquisition Setup view, click **Import**.
2. In the Open dialog box, select a sequence file (.sld, .csv, or .txt file) to import, and then click **Open**. QuickQuan imports the sequence into the sequence grid.
3. (Optional) Edit the sequence to specify a drug set for each sample.

Figure 36 shows two sequences: one for Drugset1 and one for Drugset2.

Importing Excel and Sequence Templates

Another way to import a sequence is to import an Excel template (.xls file extension) and a sequence template (.sld file extension) using the following procedures:

1. "Creating an Excel Template for the Assay" on page 59
2. "Creating a Sequence Template" on page 61
3. "Importing the Excel and Sequence Templates" on page 63

Creating an Excel Template for the Assay

The Excel template file describes the assay to be run, including the drug sets to use for each sequence in the assay, vial positions, number of samples per sequence, instrument method, processing method, and injection order. You can use multiple plates in a single sequence and specify more than one plate type.

In the Excel worksheet, you can specify the vial position for each sample. Make sure that you name the vial positions with names that are valid for your autosampler. If the autosampler supports vial validation, QuickQuan automatically validates each vial position specified in the Excel worksheet at run time.

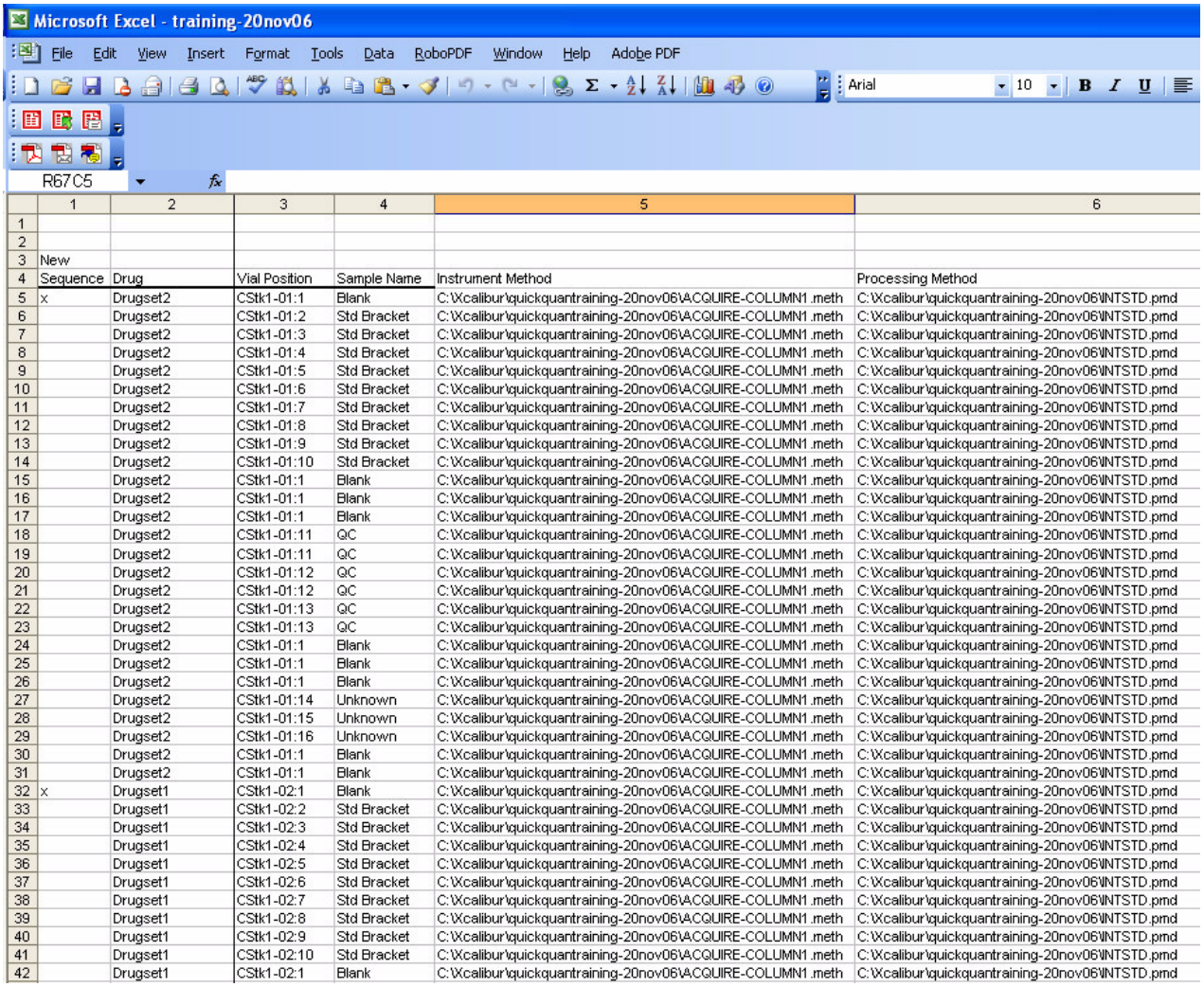
Figure 37 shows an example of an Excel template.

❖ To create the Excel template for the assay

1. In columns 2 through 6, enter the following:
   - Drug set name
   - Vial position
   - Sample name
   - Generic instrument method
   - Generic processing method

   Each row corresponds to an injection.
2. To indicate the start of a new sequence, type an **X** in column 1.
3. To indicate the end of the assay, type an **X** in column 1 in the row after the last injection. See Figure 38.
4. Save the Excel template as an .xls file.

Figure 37. Excel template for an assay


Microsoft Excel - training-20nov06

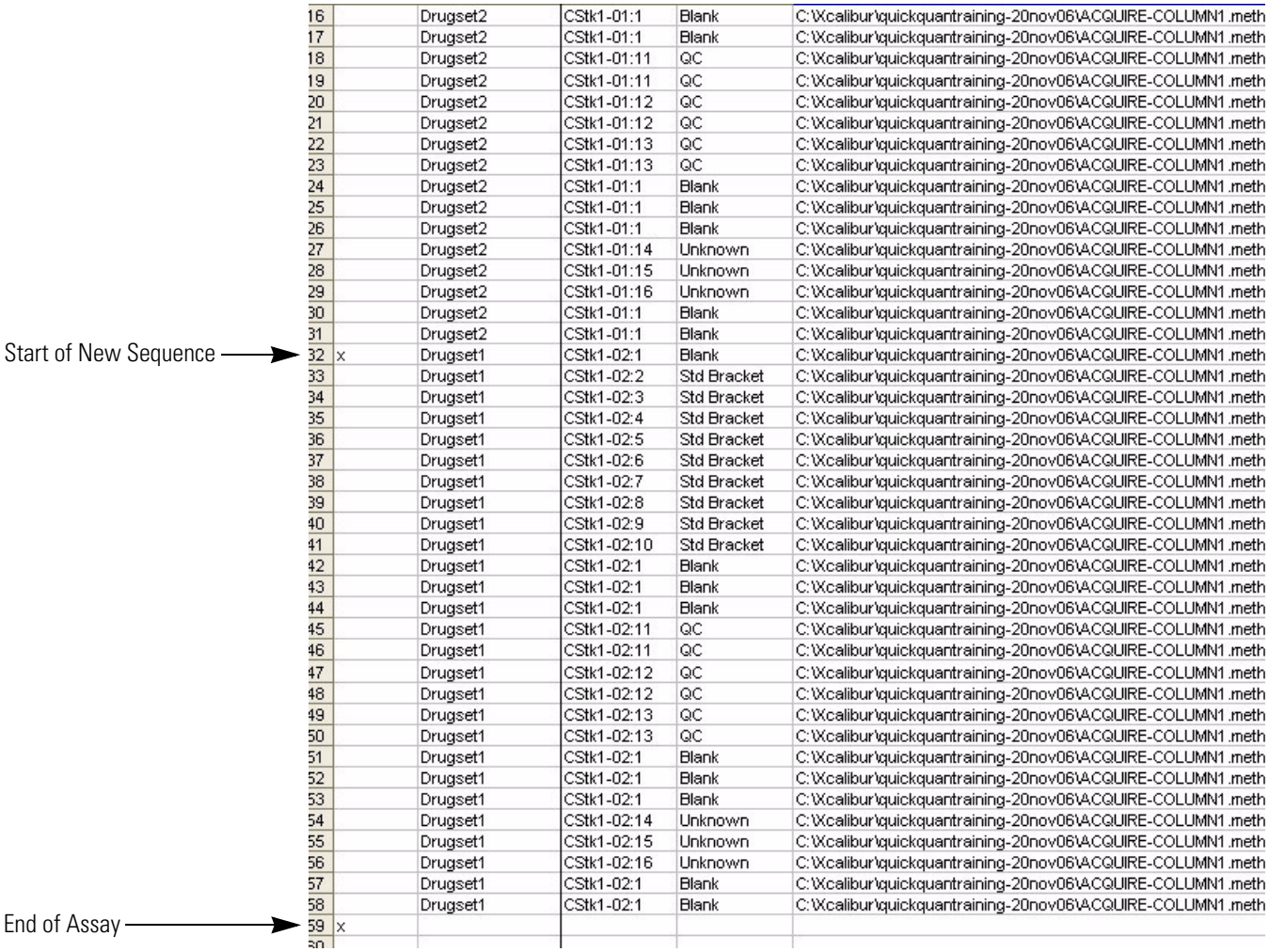
File Edit View Insert Format Tools Data RoboPDF Window Help Adobe PDF

Arial 10

R67C5

	1	2	3	4	5	6
1						
2						
3	New					
4	Sequence	Drug	Vial Position	Sample Name	Instrument Method	Processing Method
5	x	Drugset2	CStk1-01:1	Blank	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd
6		Drugset2	CStk1-01:2	Std Bracket	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd
7		Drugset2	CStk1-01:3	Std Bracket	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd
8		Drugset2	CStk1-01:4	Std Bracket	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd
9		Drugset2	CStk1-01:5	Std Bracket	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd
10		Drugset2	CStk1-01:6	Std Bracket	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd
11		Drugset2	CStk1-01:7	Std Bracket	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd
12		Drugset2	CStk1-01:8	Std Bracket	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd
13		Drugset2	CStk1-01:9	Std Bracket	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd
14		Drugset2	CStk1-01:10	Std Bracket	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd
15		Drugset2	CStk1-01:1	Blank	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd
16		Drugset2	CStk1-01:1	Blank	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd
17		Drugset2	CStk1-01:1	Blank	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd
18		Drugset2	CStk1-01:11	QC	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd
19		Drugset2	CStk1-01:11	QC	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd
20		Drugset2	CStk1-01:12	QC	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd
21		Drugset2	CStk1-01:12	QC	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd
22		Drugset2	CStk1-01:13	QC	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd
23		Drugset2	CStk1-01:13	QC	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd
24		Drugset2	CStk1-01:1	Blank	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd
25		Drugset2	CStk1-01:1	Blank	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd
26		Drugset2	CStk1-01:1	Blank	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd
27		Drugset2	CStk1-01:14	Unknown	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd
28		Drugset2	CStk1-01:15	Unknown	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd
29		Drugset2	CStk1-01:16	Unknown	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd
30		Drugset2	CStk1-01:1	Blank	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd
31		Drugset2	CStk1-01:1	Blank	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd
32	x	Drugset1	CStk1-02:1	Blank	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd
33		Drugset1	CStk1-02:2	Std Bracket	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd
34		Drugset1	CStk1-02:3	Std Bracket	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd
35		Drugset1	CStk1-02:4	Std Bracket	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd
36		Drugset1	CStk1-02:5	Std Bracket	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd
37		Drugset1	CStk1-02:6	Std Bracket	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd
38		Drugset1	CStk1-02:7	Std Bracket	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd
39		Drugset1	CStk1-02:8	Std Bracket	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd
40		Drugset1	CStk1-02:9	Std Bracket	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd
41		Drugset1	CStk1-02:10	Std Bracket	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd
42		Drugset1	CStk1-02:1	Blank	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd

Figure 38. Excel template, showing the start of a new sequence and the end of the assay



16		Drugset2	CStk1-01:1	Blank	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
17		Drugset2	CStk1-01:1	Blank	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
18		Drugset2	CStk1-01:11	QC	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
19		Drugset2	CStk1-01:11	QC	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
20		Drugset2	CStk1-01:12	QC	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
21		Drugset2	CStk1-01:12	QC	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
22		Drugset2	CStk1-01:13	QC	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
23		Drugset2	CStk1-01:13	QC	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
24		Drugset2	CStk1-01:1	Blank	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
25		Drugset2	CStk1-01:1	Blank	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
26		Drugset2	CStk1-01:1	Blank	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
27		Drugset2	CStk1-01:14	Unknown	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
28		Drugset2	CStk1-01:15	Unknown	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
29		Drugset2	CStk1-01:16	Unknown	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
30		Drugset2	CStk1-01:1	Blank	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
31		Drugset2	CStk1-01:1	Blank	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
32	x	Drugset1	CStk1-02:1	Blank	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
33		Drugset1	CStk1-02:2	Std Bracket	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
34		Drugset1	CStk1-02:3	Std Bracket	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
35		Drugset1	CStk1-02:4	Std Bracket	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
36		Drugset1	CStk1-02:5	Std Bracket	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
37		Drugset1	CStk1-02:6	Std Bracket	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
38		Drugset1	CStk1-02:7	Std Bracket	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
39		Drugset1	CStk1-02:8	Std Bracket	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
40		Drugset1	CStk1-02:9	Std Bracket	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
41		Drugset1	CStk1-02:10	Std Bracket	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
42		Drugset1	CStk1-02:1	Blank	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
43		Drugset1	CStk1-02:1	Blank	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
44		Drugset1	CStk1-02:1	Blank	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
45		Drugset1	CStk1-02:11	QC	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
46		Drugset1	CStk1-02:11	QC	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
47		Drugset1	CStk1-02:12	QC	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
48		Drugset1	CStk1-02:12	QC	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
49		Drugset1	CStk1-02:13	QC	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
50		Drugset1	CStk1-02:13	QC	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
51		Drugset1	CStk1-02:1	Blank	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
52		Drugset1	CStk1-02:1	Blank	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
53		Drugset1	CStk1-02:1	Blank	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
54		Drugset1	CStk1-02:14	Unknown	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
55		Drugset1	CStk1-02:15	Unknown	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
56		Drugset1	CStk1-02:16	Unknown	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
57		Drugset1	CStk1-02:1	Blank	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
58		Drugset1	CStk1-02:1	Blank	C:\Xcalibur\quickquantraining-20nov06\ACQUIRE-COLUMN1.meth
59	x				

Creating a Sequence Template

The sequence template (.sld file) is a generic sequence to be run for the entire assay. The sequence template must correspond to the Excel template. You create the sequence template in the Xcalibur Home Page window – Sequence Setup view. See the Xcalibur Help for details on how to create the sequence in the Sequence Setup view.

The sequence template specifies the following:

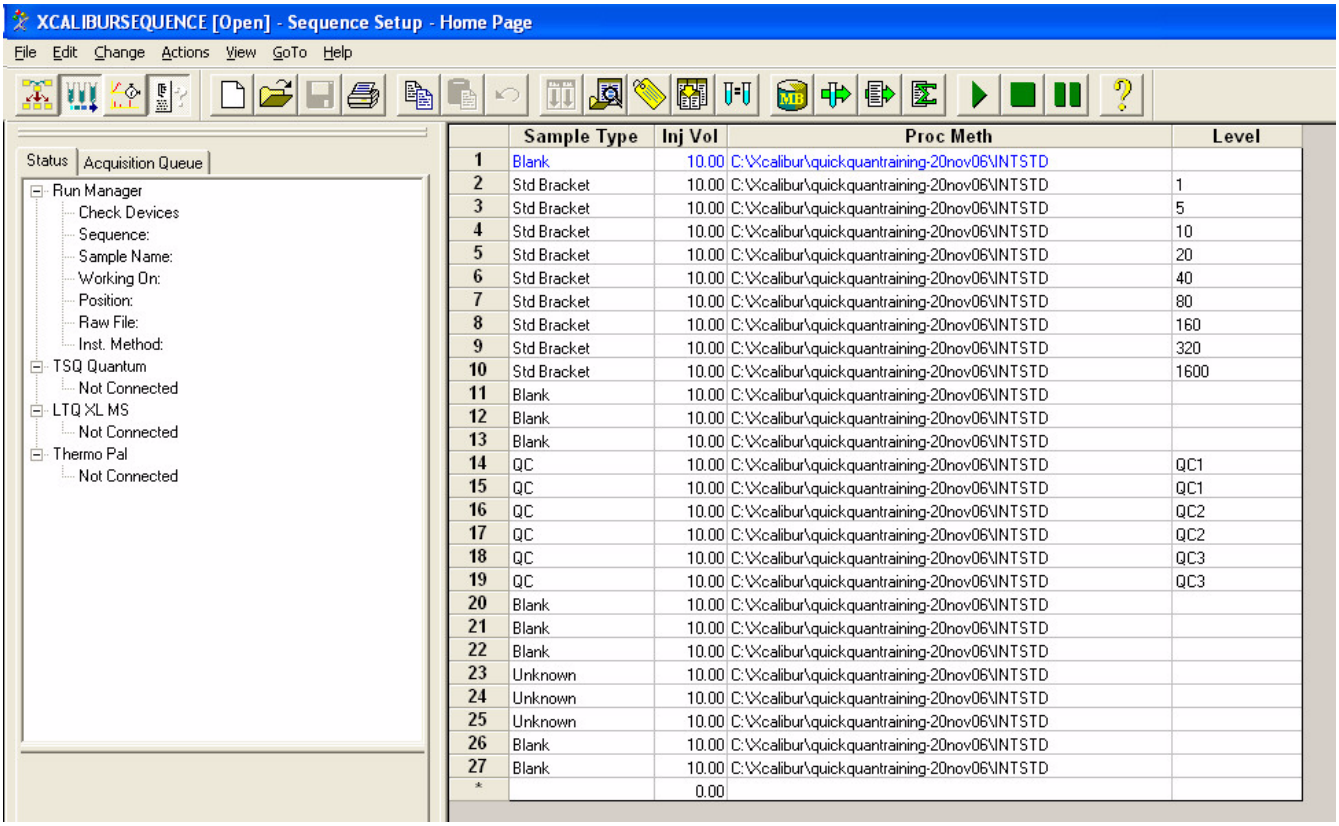
- Sample injection type
- Injection volume used for each sample
- Arrangement of sample types (standards, QCs, blanks, and unknowns)

At run time, QuickQuan replaces the drug set name, vial position, instrument method, processing method, and sample name with the information specified in the Excel template for each sequence in the assay.

IMPORTANT The number of samples in the selected sequence template (.sld file) must match the number of samples in each sequence of the selected Excel assay layout template (.xls file).

The number of samples in the selected sequence template must match the number of samples in each sequence of the Excel template file selected. For example, the sequence template file shown in Figure 39 corresponds to the Excel template shown in Figure 37. In this example, 27 samples must be defined in the sequence template, because the Excel template has 27 samples per drug set. This sequence is specified only once, and QuickQuan refers back to it multiple times.

Figure 39. Sequence template corresponding to the Excel template in Figure 37



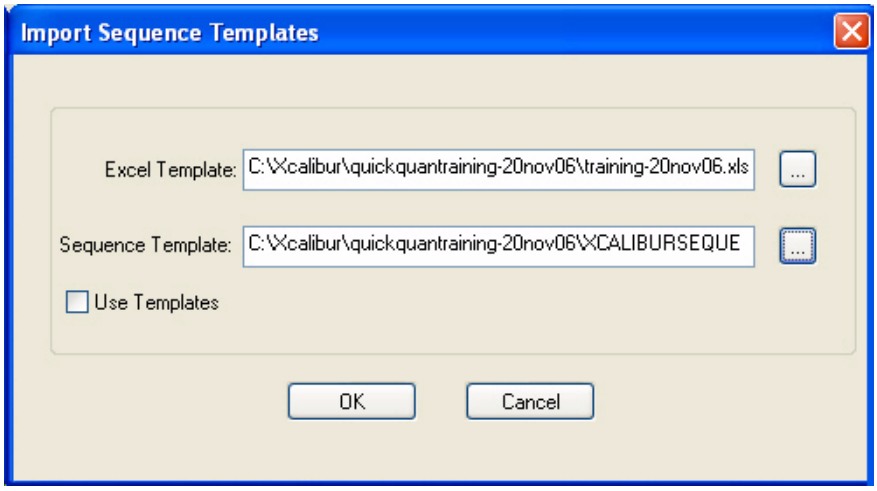
	Sample Type	Inj Vol	Proc Meth	Level
1	Blank	10.00	C:\Xcalibur\quickquantraining-20nov06\INTSTD	
2	Std Bracket	10.00	C:\Xcalibur\quickquantraining-20nov06\INTSTD	1
3	Std Bracket	10.00	C:\Xcalibur\quickquantraining-20nov06\INTSTD	5
4	Std Bracket	10.00	C:\Xcalibur\quickquantraining-20nov06\INTSTD	10
5	Std Bracket	10.00	C:\Xcalibur\quickquantraining-20nov06\INTSTD	20
6	Std Bracket	10.00	C:\Xcalibur\quickquantraining-20nov06\INTSTD	40
7	Std Bracket	10.00	C:\Xcalibur\quickquantraining-20nov06\INTSTD	80
8	Std Bracket	10.00	C:\Xcalibur\quickquantraining-20nov06\INTSTD	160
9	Std Bracket	10.00	C:\Xcalibur\quickquantraining-20nov06\INTSTD	320
10	Std Bracket	10.00	C:\Xcalibur\quickquantraining-20nov06\INTSTD	1600
11	Blank	10.00	C:\Xcalibur\quickquantraining-20nov06\INTSTD	
12	Blank	10.00	C:\Xcalibur\quickquantraining-20nov06\INTSTD	
13	Blank	10.00	C:\Xcalibur\quickquantraining-20nov06\INTSTD	
14	QC	10.00	C:\Xcalibur\quickquantraining-20nov06\INTSTD	QC1
15	QC	10.00	C:\Xcalibur\quickquantraining-20nov06\INTSTD	QC1
16	QC	10.00	C:\Xcalibur\quickquantraining-20nov06\INTSTD	QC2
17	QC	10.00	C:\Xcalibur\quickquantraining-20nov06\INTSTD	QC2
18	QC	10.00	C:\Xcalibur\quickquantraining-20nov06\INTSTD	QC3
19	QC	10.00	C:\Xcalibur\quickquantraining-20nov06\INTSTD	QC3
20	Blank	10.00	C:\Xcalibur\quickquantraining-20nov06\INTSTD	
21	Blank	10.00	C:\Xcalibur\quickquantraining-20nov06\INTSTD	
22	Blank	10.00	C:\Xcalibur\quickquantraining-20nov06\INTSTD	
23	Unknown	10.00	C:\Xcalibur\quickquantraining-20nov06\INTSTD	
24	Unknown	10.00	C:\Xcalibur\quickquantraining-20nov06\INTSTD	
25	Unknown	10.00	C:\Xcalibur\quickquantraining-20nov06\INTSTD	
26	Blank	10.00	C:\Xcalibur\quickquantraining-20nov06\INTSTD	
27	Blank	10.00	C:\Xcalibur\quickquantraining-20nov06\INTSTD	
*		0.00		

Importing the Excel and Sequence Templates

❖ To import an Excel template and sequence template

1. Choose **File > Import Acquisition Sequence > From Templates** to open the Import Sequence Templates dialog box. See Figure 40.

   Figure 40. Import Sequence Templates dialog box

2. Select the Excel template and sequence template.
3. Click **OK** to close the dialog box.

Saving the QuickQuan Assay

You save the QuickQuan assay in an .aql file.

❖ To save the QuickQuan assay

1. Choose **File > Save As** to open the Save As dialog box.
2. Enter a name for the assay in the File Name box.
3. Click **Save** to save the assay.

Running an Acquisition

Before running an assay, QuickQuan can optimize either all the compounds in the assay, or only the unoptimized compounds that are not in the optimization database.

❖ To prepare to run an acquisition

1. Open Xcalibur to the Real Time Plot view.
2. In Xcalibur, verify that devices are ready, and make sure the initial system parameters are within the acceptable ranges.
3. Verify that the vessel holding the compounds for tuning is ready and in position. Verify the same for assay plates.
4. Start Quantum EZ Tune.

❖ To display the Configuration Options dialog box

In the QuickQuan navigation pane, click **Acquisition**, and then click **Go**.

❖ To set up and run the acquisition

1. In the Configuration Options dialog box (Figure 41), select **High-Throughput Acquisition** to run an analytical experiment with real-time compound optimization.
2. (Optional) To use optimization information that is already in the database, select the **Use Optimization Database for Existing Compounds** check box. QuickQuan optimizes the compounds that are in the tune plate that have not been optimized.

   If the check box is cleared, QuickQuan optimizes all compounds that are in the tune plate.

3. In the Instrument Settings area, verify the following:
   a. The Instrument column lists only the required instruments.

      If the required instruments do not appear, see "Configuring and Setting Up Instruments" on page 79. You must configure the instruments before performing the following steps.

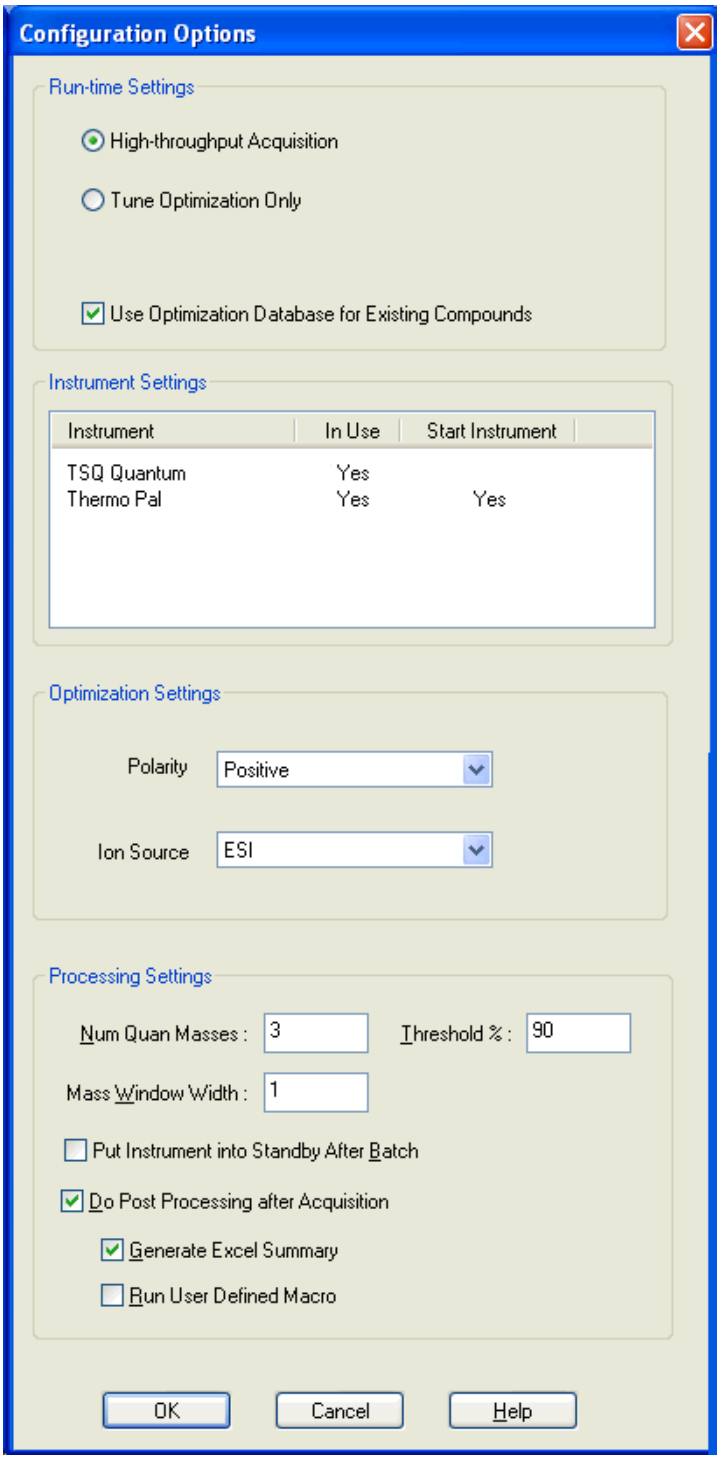
   b. The In Use column displays a **Yes** for each instrument. Click the **In Use** cell to toggle on or off the **Yes**.

   c. (Optional) The **Start Instrument** cell displays **Yes** for the instrument that will initiate the run.

4. In the Optimization Settings area, select the following:
   a. **Polarity**: positive, negative, or both

   b. **Ion source**: ESI, APCI, APPI, or H-ESI

Figure 41. Configuration Options dialog box



5. In the Num Quan Masses box, type the number of masses to use for post acquisition processing. The valid range is 1 to 3.
6. In the Threshold **%** box, type a percentage. All the Num Quan Masses selected for post processing must meet the specified percentage threshold of the highest intensity ion.
7. (Optional) To set the devices to standby after the acquisition has finished, select the **Put Instrument Into Standby Mode After Batch** check box.
8. (Optional) To start post-processing after each sequence has been acquired, select the **Do Post Processing After Acquisition** check box.

   You can also select the following options:

   a. To produce a summary report for the acquisition data after post processing has completed, select the **Generate Excel Summary** check box.

   b. To execute a custom Excel macro after data acquisition and post processing have finished, select the **Run User Defined Macro** check box. (For details, see "Using a Macro To Perform Custom Calculations" on page 83.)
9. Click **OK** to start the acquisition. QuickQuan displays the Acquisition Status view. See Figure 42.

You can view the status of the run in the EZ Tune Real Time Plot view or in the QuickQuan Acquisition Status view or both.

When you run the acquisition, QuickQuan creates a time and date stamped folder under the folder you specified as the output path (Figure 35 on page 54). In the output path folder, QuickQuan creates a folder for each drug set (01_Drugset2 and 02_Drugset1). QuickQuan puts the raw and processed data in the drug set folders. See Figure 43.

Figure 42. Acquisition Status view

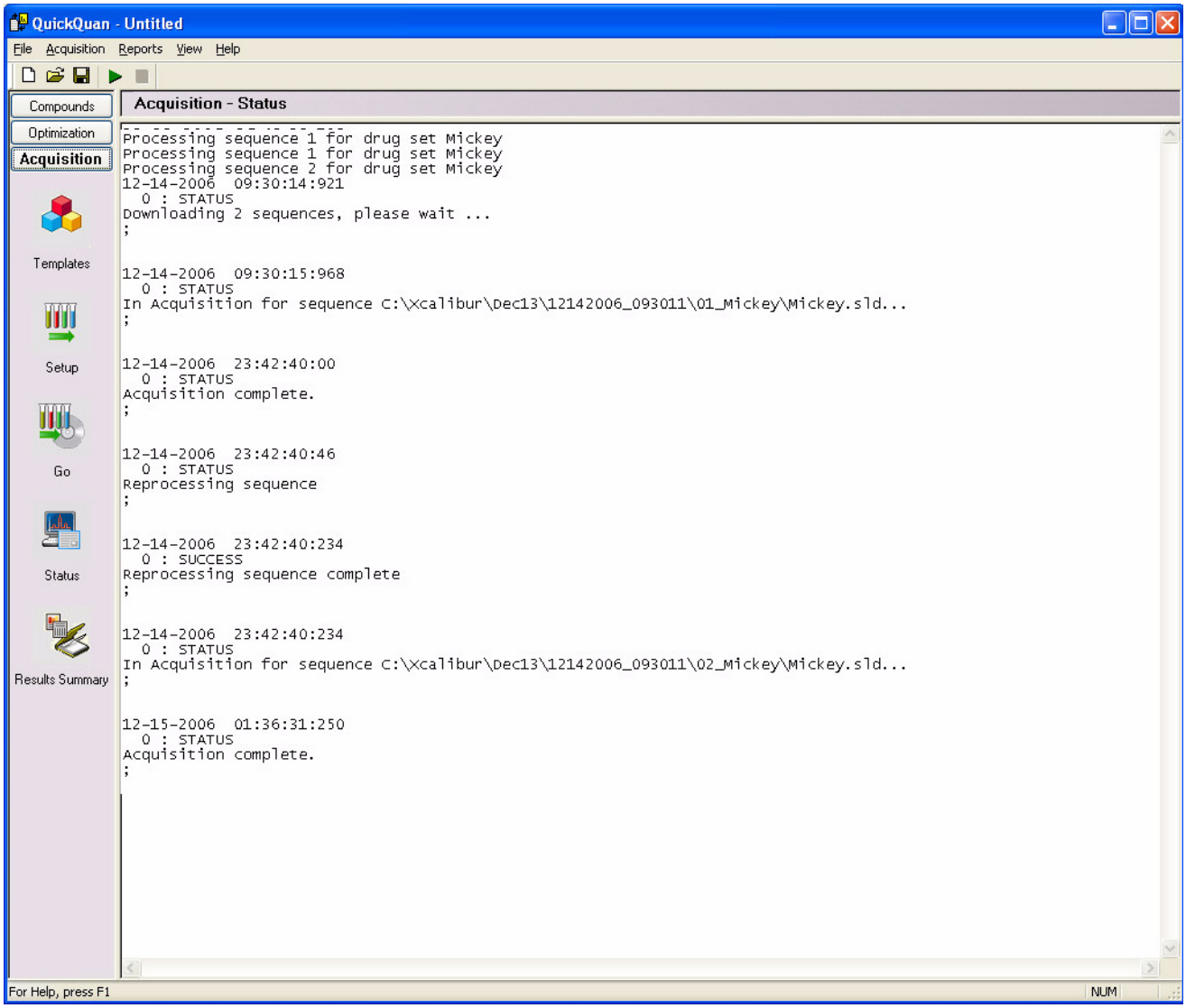
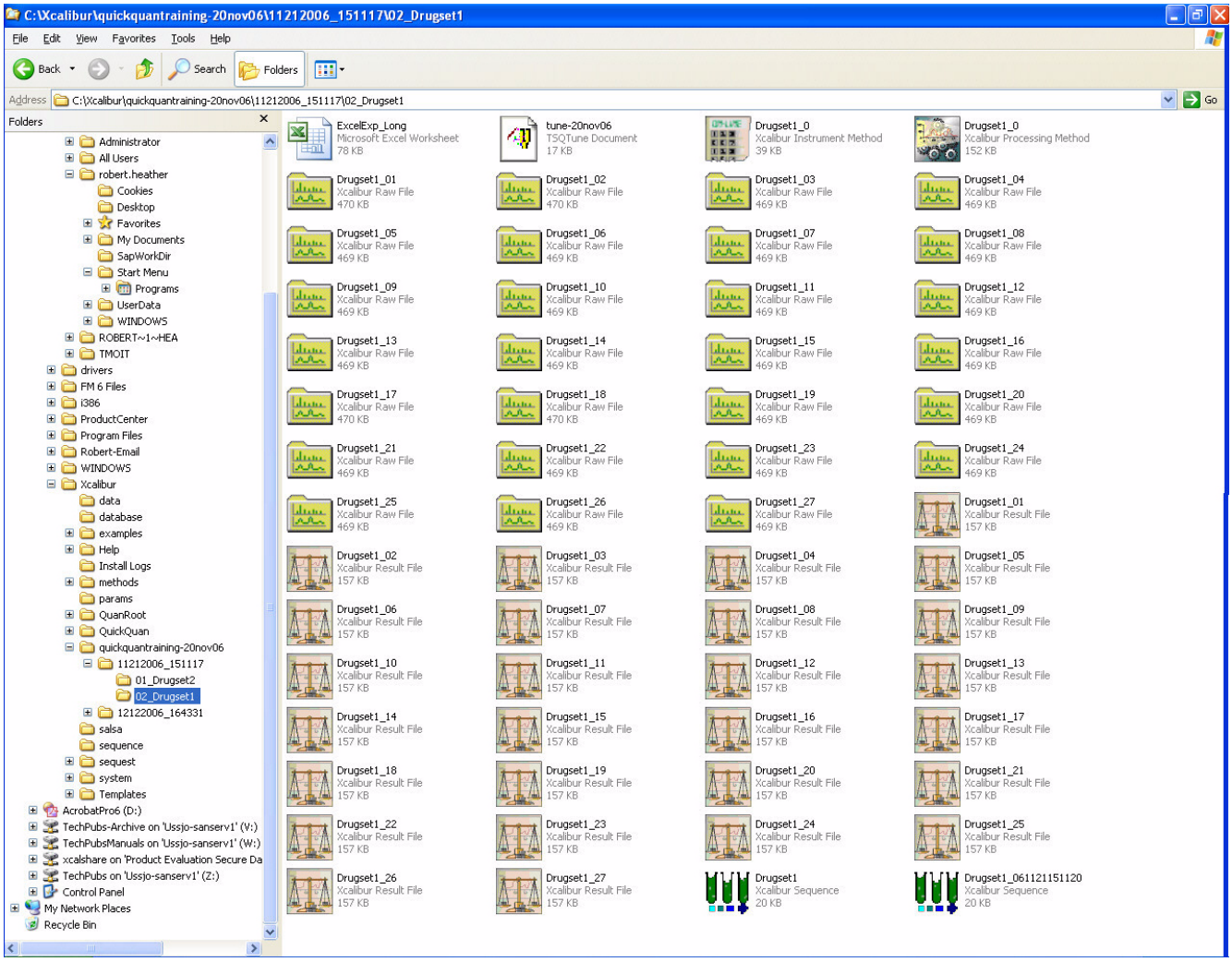


Figure 43. Time and date stamped folder location of raw files, result files, and Excel acquisition file



Stopping an Acquisition

❖ **To stop an acquisition before the run is finished**

On the QuickQuan toolbar, click .

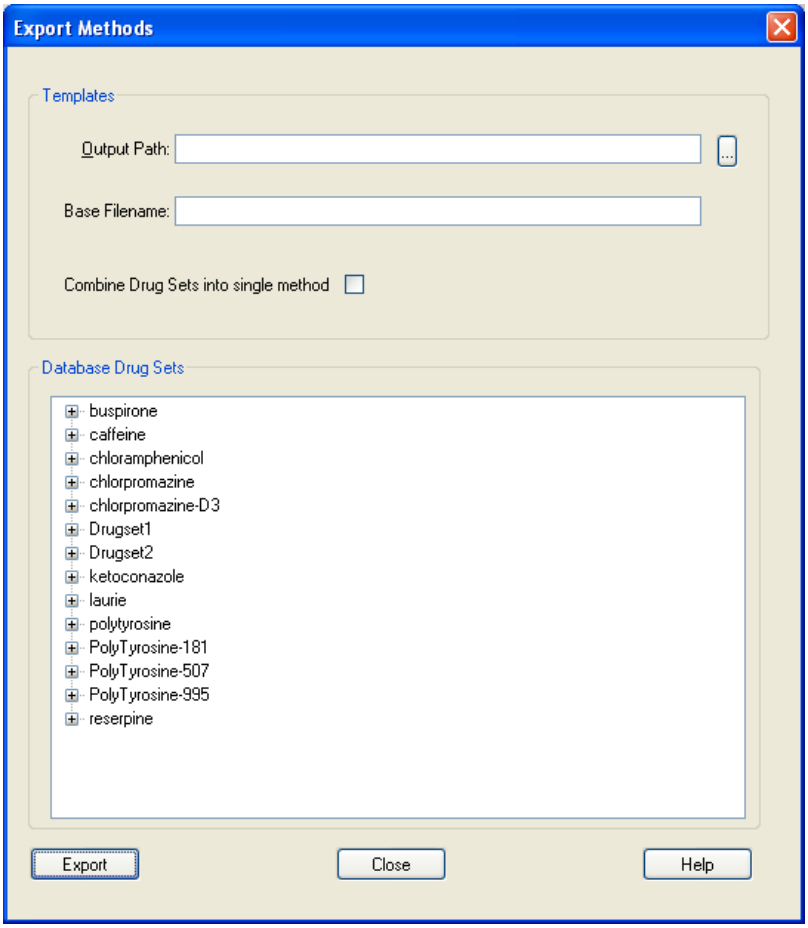
Exporting the Instrument and Processing Methods

You can export the generic instrument method (.meth) and processing method (.pmd) from the Acquisition Templates view for use with other applications.

❖ **To export the methods**

1. In the Acquisition Templates view, specify the template information. See "Specifying Template Options" on page 53.
2. Choose **File > Export Methods**. The Export Methods dialog box appears.

Figure 44. Export Methods dialog box



3. In the Output Path box, specify the file path for the exported files.
4. In the Base Filename box, type the file name.
5. To create a single instrument method and processing method for all the selected drug sets, select the **Combine Drug Sets into single method** check box.

   Clear the check box if you want to create a separate instrument method and processing method for each selected drug set.
6. In the Database Drug Sets list, select the drug sets and compounds for the exported methods. To select multiple drug sets, press CTRL+click.
7. Click **Export**. QuickQuan creates a time-stamped folder at the specified output path and stores the instrument method and processing method for the selected drug sets in that folder.

Reviewing the Results

This chapter describes how to display QuickQuan results.

Contents

- Reviewing Quantitation Results
- Generating and Viewing the Acquisition Summary Report
- How QuickQuan Performs Post Processing

Reviewing Quantitation Results

Use the Acquisition Results Summary view to display and review the quantitation results.

❖ To display the Acquisition Results Summary view

In the QuickQuan navigation pane, click **Acquisition**, and then click **Results Summary**. The Acquisition – Results Summary view appears.

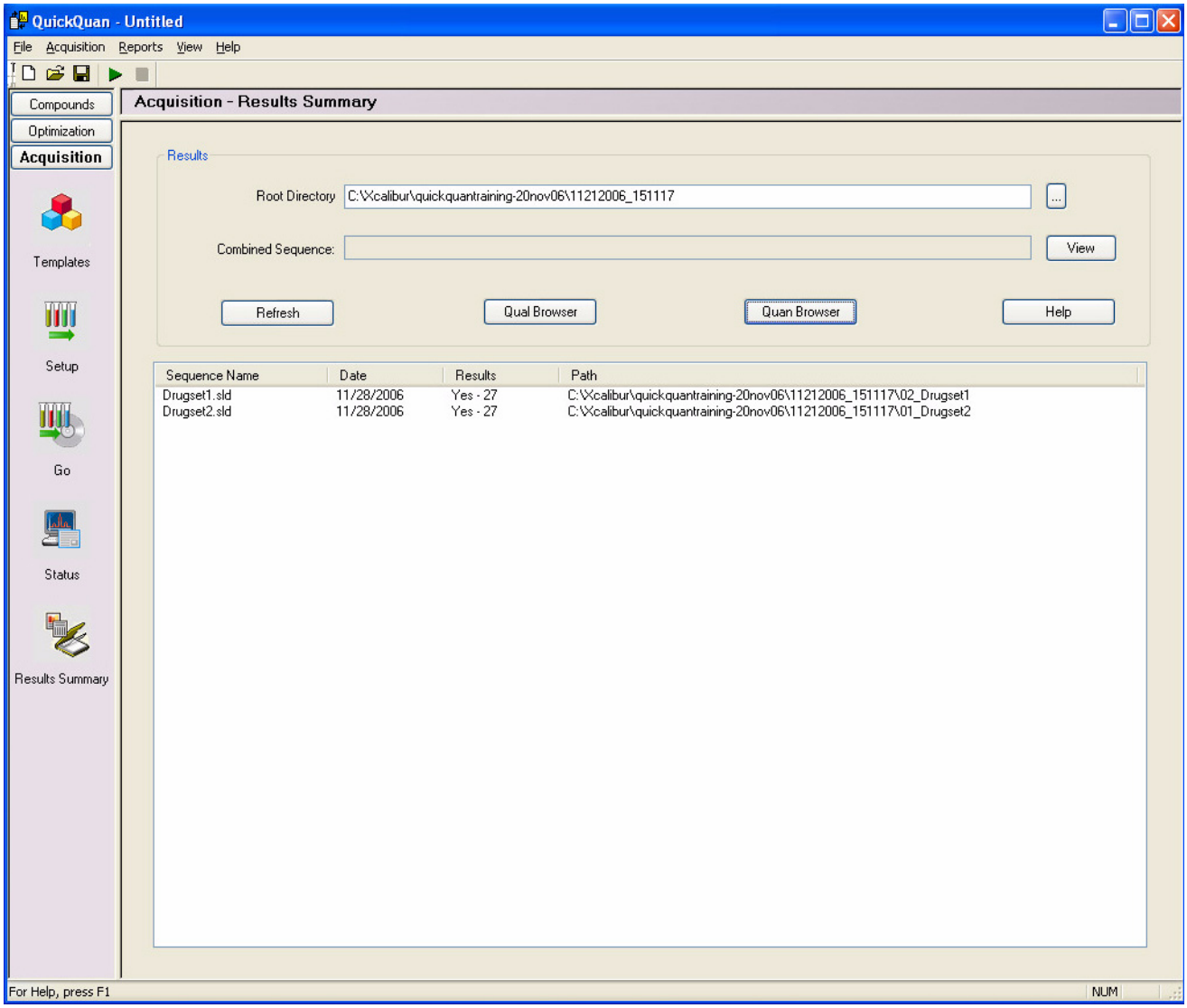
❖ To display and review the quantitation results

1. In the Root Directory box, browse to and select the time and date stamped folder that QuickQuan created, for example:

   <your_output_path_folder><timestamp_folder_for_selected_acquisition>

   See Figure 45.

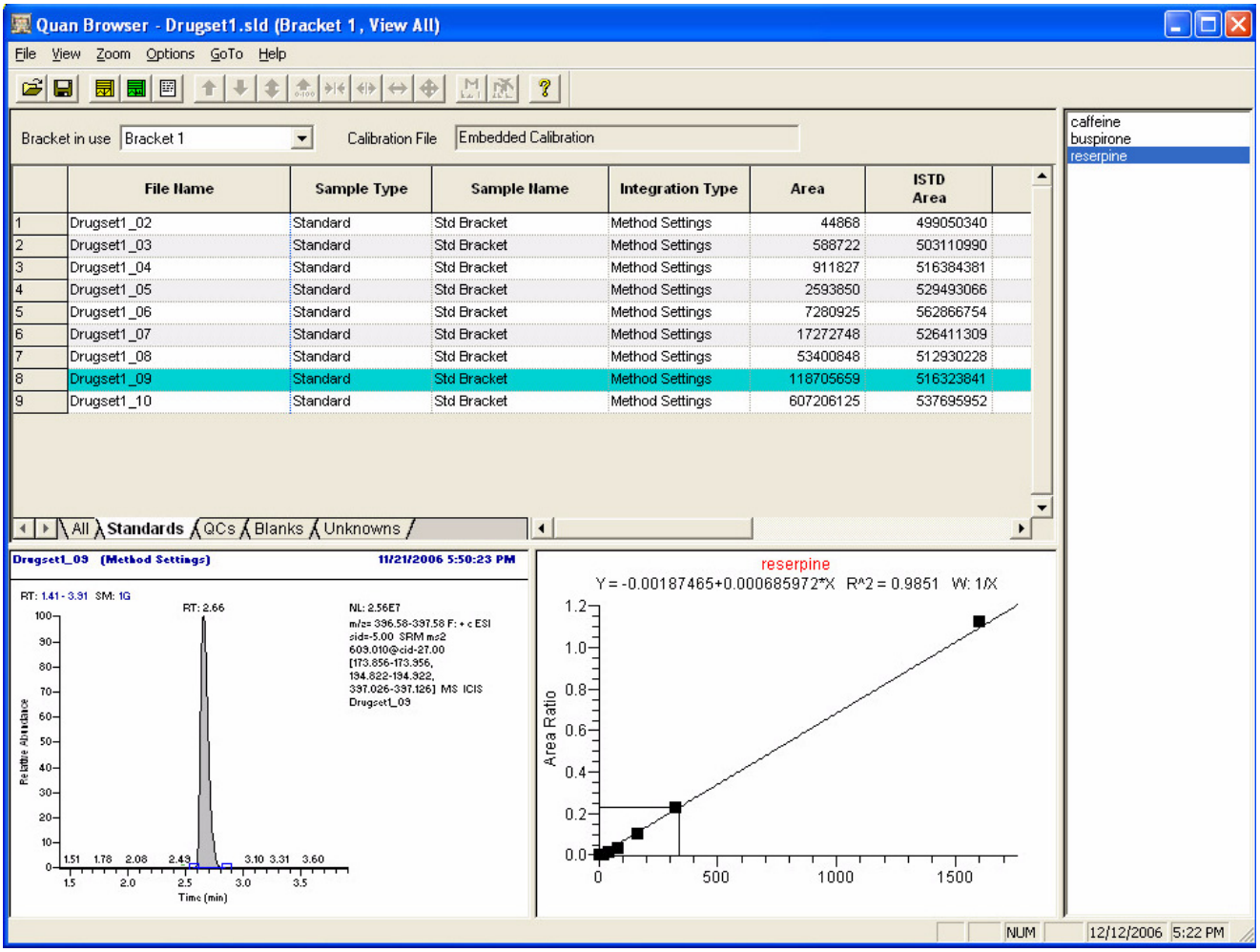
Figure 45. Acquisition Results Summary view



2. Click **Quan Browser**. Xcalibur Quan Browser starts and displays the data in the Quan Browser window. See Figure 46.

3. Select a component to display the results.

Figure 46. Quan Browser, showing the results for reserpine


Quan Browser - Drugset1.sld (Bracket 1, View All)
File View Zoom Options GoTo Help
Bracket in use Bracket 1
Calibration File Embedded Calibration
caffeine
buspirone
reserpine
File Name | Sample Type | Sample Name | Integration Type | Area | ISTD Area
1 Drugset1_02 Standard Std Bracket Method Settings 44868 499050340
2 Drugset1_03 Standard Std Bracket Method Settings 588722 503110990
3 Drugset1_04 Standard Std Bracket Method Settings 911827 516384381
4 Drugset1_05 Standard Std Bracket Method Settings 2593850 529493066
5 Drugset1_06 Standard Std Bracket Method Settings 7280925 562866754
6 Drugset1_07 Standard Std Bracket Method Settings 17272748 526411309
7 Drugset1_08 Standard Std Bracket Method Settings 53400848 512930228
8 Drugset1_09 Standard Std Bracket Method Settings 118705659 516323841
9 Drugset1_10 Standard Std Bracket Method Settings 607206125 537695952
All Standards QCs Blanks Unknowns
Drugset1_09 (Method Settings) 11/21/2006 5:50:23 PM
RT: 2.66
Relative Abundance
Time (min)
reserpine
Y = -0.00187465+0.000685972*X R^2 = 0.9851 W: 1/X
Area Ratio
NUM 12/12/2006 5:22 PM

Generating and Viewing the Acquisition Summary Report

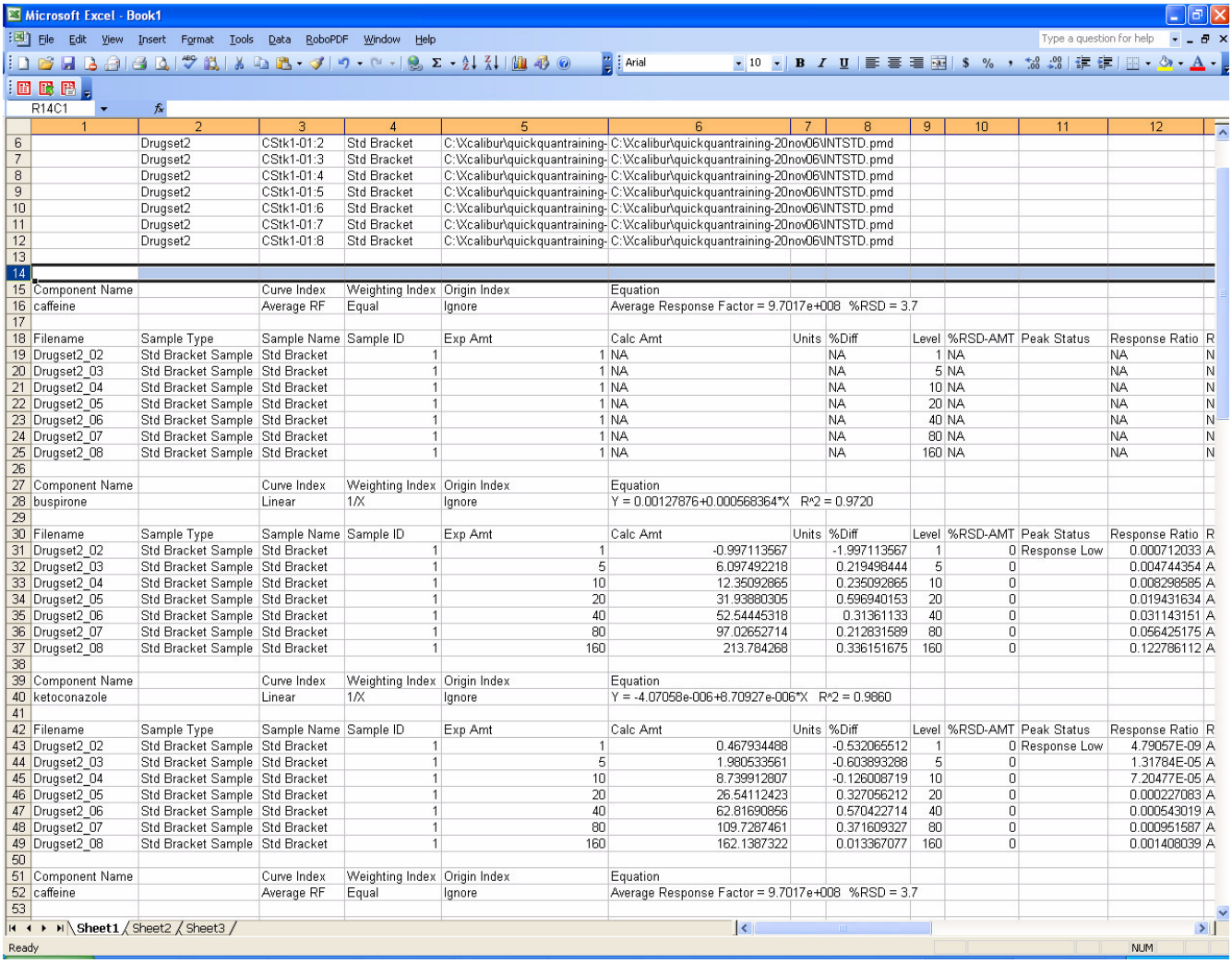
QuickQuan compiles the individual sample acquisition reports into a summary report (.xls file) that you can open using Excel.

The Acquisition Summary Report contains the following data:

- File name
- Sample type, name, and ID
- Expected and calculated amount
- Units
- %Diff
- Level
- %RSD
- Peak status
- Response
- Area
- Height
- ISTD area and height
- Retention time (RT), Rel RT, Del RT
- Signal-to-noise ratio (S/N)
- Start and end time
- Start and end height
- Integ code
- Search window
- Threshold
- Smoothing
- Acquisition date
- Duration
- Exp method
- PMD method
- Vial
- Injection volume
- Sample weight and volume
- ISTD base amount and calc amt
- Dilution factor

Figure 47 shows an example of an acquisition summary report.

Figure 47. Excel acquisition summary report



Microsoft Excel - Book1

	1	2	3	4	5	6	7	8	9	10	11	12
6		Drugset2	CStk1-01:2	Std Bracket	C:\Xcalibur\quickquantraining-	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd						
7		Drugset2	CStk1-01:3	Std Bracket	C:\Xcalibur\quickquantraining-	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd						
8		Drugset2	CStk1-01:4	Std Bracket	C:\Xcalibur\quickquantraining-	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd						
9		Drugset2	CStk1-01:5	Std Bracket	C:\Xcalibur\quickquantraining-	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd						
10		Drugset2	CStk1-01:6	Std Bracket	C:\Xcalibur\quickquantraining-	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd						
11		Drugset2	CStk1-01:7	Std Bracket	C:\Xcalibur\quickquantraining-	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd						
12		Drugset2	CStk1-01:8	Std Bracket	C:\Xcalibur\quickquantraining-	C:\Xcalibur\quickquantraining-20nov06\INTSTD.pmd						
13												
14												
15	Component Name		Curve Index	Weighting Index	Origin Index	Equation						
16	caffeine		Average RF	Equal	Ignore	Average Response Factor = 9.7017e+008 %RSD = 3.7						
17												
18	Filename	Sample Type	Sample Name	Sample ID	Exp Amt	Calc Amt	Units	%Diff	Level	%RSD-AMT	Peak Status	Response Ratio
19	Drugset2_02	Std Bracket Sample	Std Bracket	1	1	NA		NA	1	NA		NA
20	Drugset2_03	Std Bracket Sample	Std Bracket	1	1	NA		NA	5	NA		NA
21	Drugset2_04	Std Bracket Sample	Std Bracket	1	1	NA		NA	10	NA		NA
22	Drugset2_05	Std Bracket Sample	Std Bracket	1	1	NA		NA	20	NA		NA
23	Drugset2_06	Std Bracket Sample	Std Bracket	1	1	NA		NA	40	NA		NA
24	Drugset2_07	Std Bracket Sample	Std Bracket	1	1	NA		NA	80	NA		NA
25	Drugset2_08	Std Bracket Sample	Std Bracket	1	1	NA		NA	160	NA		NA
26												
27	Component Name		Curve Index	Weighting Index	Origin Index	Equation						
28	buspirone		Linear	1/X	Ignore	Y = 0.00127876+0.000568364*X R^2 = 0.9720						
29												
30	Filename	Sample Type	Sample Name	Sample ID	Exp Amt	Calc Amt	Units	%Diff	Level	%RSD-AMT	Peak Status	Response Ratio
31	Drugset2_02	Std Bracket Sample	Std Bracket	1	1	-0.997113567		-1.997113567	1	0	Response Low	0.000712033
32	Drugset2_03	Std Bracket Sample	Std Bracket	1	5	6.097492218		0.219498444	5	0		0.004744354
33	Drugset2_04	Std Bracket Sample	Std Bracket	1	10	12.35092865		0.235092865	10	0		0.008298585
34	Drugset2_05	Std Bracket Sample	Std Bracket	1	20	31.93880305		0.596940153	20	0		0.019431634
35	Drugset2_06	Std Bracket Sample	Std Bracket	1	40	52.54445318		0.31361133	40	0		0.031143151
36	Drugset2_07	Std Bracket Sample	Std Bracket	1	80	97.02652714		0.212831589	80	0		0.056425175
37	Drugset2_08	Std Bracket Sample	Std Bracket	1	160	213.784268		0.336151675	160	0		0.122786112
38												
39	Component Name		Curve Index	Weighting Index	Origin Index	Equation						
40	ketoconazole		Linear	1/X	Ignore	Y = -4.07058e-006+8.70927e-006*X R^2 = 0.9860						
41												
42	Filename	Sample Type	Sample Name	Sample ID	Exp Amt	Calc Amt	Units	%Diff	Level	%RSD-AMT	Peak Status	Response Ratio
43	Drugset2_02	Std Bracket Sample	Std Bracket	1	1	0.467934488		-0.532065512	1	0	Response Low	4.79057E-09
44	Drugset2_03	Std Bracket Sample	Std Bracket	1	5	1.980533561		-0.603893288	5	0		1.31784E-05
45	Drugset2_04	Std Bracket Sample	Std Bracket	1	10	8.739912807		-0.126008719	10	0		7.20477E-05
46	Drugset2_05	Std Bracket Sample	Std Bracket	1	20	26.54112423		0.327056212	20	0		0.000227083
47	Drugset2_06	Std Bracket Sample	Std Bracket	1	40	62.81690856		0.570422714	40	0		0.000543019
48	Drugset2_07	Std Bracket Sample	Std Bracket	1	80	109.7287461		0.371609327	80	0		0.000951587
49	Drugset2_08	Std Bracket Sample	Std Bracket	1	160	162.1387322		0.013367077	160	0		0.001408039
50												
51	Component Name		Curve Index	Weighting Index	Origin Index	Equation						
52	caffeine		Average RF	Equal	Ignore	Average Response Factor = 9.7017e+008 %RSD = 3.7						
53												

Sheet1 / Sheet2 / Sheet3

Ready NUM

❖ To generate an acquisition summary report

1. In the QuickQuan window, choose **Reports > Acquisition Summary Report**. The Browse for Folder dialog box appears.
2. Select the destination folder, and then click **OK**, for example:

   <your_output_path_folder><timestamp_folder_for_selected_acquisition>

QuickQuan creates a Microsoft Excel file (.xls) that combines every Xcalibur summary report for each sequence of the assay into a single acquisition summary report.

❖ To view an acquisition summary report

In Microsoft Excel, open the Excel template file for the assay. The file is in the folder that contains the files for the assay of interest.

How QuickQuan Performs Post Processing

To obtain post-processed data, you must specify the configuration settings for post processing before running the acquisition.

If you have configured the post-processing option, QuickQuan does the following:

1. Submits the acquired sequence to the Xcalibur data system.
2. Monitors the acquisition files being generated for each sequence that is submitted, and performs the back-end processing that communicates with Xcalibur. At the completion of each sequence, QuickQuan attempts to post process the sequence using the information about each compound assigned to the drug sets for each sequence.
3. Determines the required expected retention time (RT) for each component in the processing method. QuickQuan determines this value by extracting the filtered mass chromatogram specified for each component, using the most concentrated calibrant level as specified in the processing method (.meth file). QuickQuan uses the most intense data point as the expected RT and enters it in the processing method for that component.
4. Enables you to specify from one to three masses to be selected when the component specifications in the processing method are created. Only the one to three product ions with the greatest intensity are used in the quantification of the component. QuickQuan selects these masses from the scan corresponding to the expected RT determined above. The top ions are selected only from those whose intensities are greater than the user-defined threshold of the intensity of the base peak for the scan.
5. Instructs Xcalibur to reprocess the sequence with the new processing modifications when the component modification process is complete.

Configuration Procedures

This appendix includes configuration procedures that you might need to use periodically.

Contents

- Configuring and Setting Up Instruments
- Configuring and Setting Up Instruments for Aria
- Bypassing the LC Column and the Dual-Pump, Dual-Column Configuration

Configuring and Setting Up Instruments

If you are running QuickQuan with Aria OS, see "Configuring and Setting Up Instruments for Aria" on page 80.

❖ **To configure and set up the instruments**

1. Close QuickQuan, Quantum Tune, and Xcalibur.
2. On the Windows desktop, click the **Instrument Configuration** shortcut to start the Instrument Configuration software.
3. In the Instrument Configuration window, configure the following instruments:
   - LC pump
   - Autosampler
   - TSQ Quantum

   Click **Done**.
4. Start QuickQuan. In the QuickQuan window, choose **Acquisition > Configuration**.
5. In the Configuration Options dialog box, select **Tune Optimization Only**.
6. In the Instrument Settings area, specify the following:
   - TSQ Quantum, LC pump, and autosampler are in use. (Yes appears in the In Use column.)
   - Autosampler is set to start. (Yes appears in the Start Instrument column.)
7. Click **OK**.

Configuring and Setting Up Instruments for Aria

If you have Aria OS installed, you can use the following procedure to configure and set up the instruments for optimization. For more information on running QuickQuan with Aria, see the *QuickQuan and Aria Quick Start*.

❖ To configure and set up the instruments for the Aria workflow

1. Open the Instrument Configuration and Settings dialog box as follows:

   In the QuickQuan navigation pane, click **Optimization**, and then click **Instrument**.

2. In the Instrument Settings area, verify the following:

   - Only the TSQ Quantum, LC pump, and autosampler are configured. (The In Use column displays Yes for each instrument.)
   - The autosampler is set to start. (The Start Instrument column displays Yes.)
   - The Status column displays Ready to Download for each instrument.

   If the instrument settings are correct, click **OK**. Otherwise, continue with step 3.

3. To reconfigure the instruments, do the following:

   IMPORTANT Before starting Instrument Configuration, verify that Aria, Quantum Tune, and Xcalibur are closed.

   a. In the Instrument Configuration and Settings dialog box, click **Instrument Configuration**. The Instrument Configuration software starts.

   b. In the Instrument Configuration window, reconfigure the instruments and click **Done**.

   c. In Instrument Configuration and Settings dialog box, click **Refresh**.

   d. In the Instrument Settings area, click the **In Use** or the **Start Instrument** cell to toggle on or off the Yes for an instrument.

   e. Wait for the Status column to display **Ready to Download**.

   (Make sure the instruments have been turned on. From Xcalibur Home Page, choose **Actions > Devices On**.)

4. In the Instrument Configuration and Settings dialog box, click **OK**.

Bypassing the LC Column and the Dual-Pump, Dual-Column Configuration

You can bypass the chromatography column during optimization, and have the samples infused directly into the ion source. This option requires a Thermo Pal autosampler with multiple injection ports, multiple valves, and a stream selector.

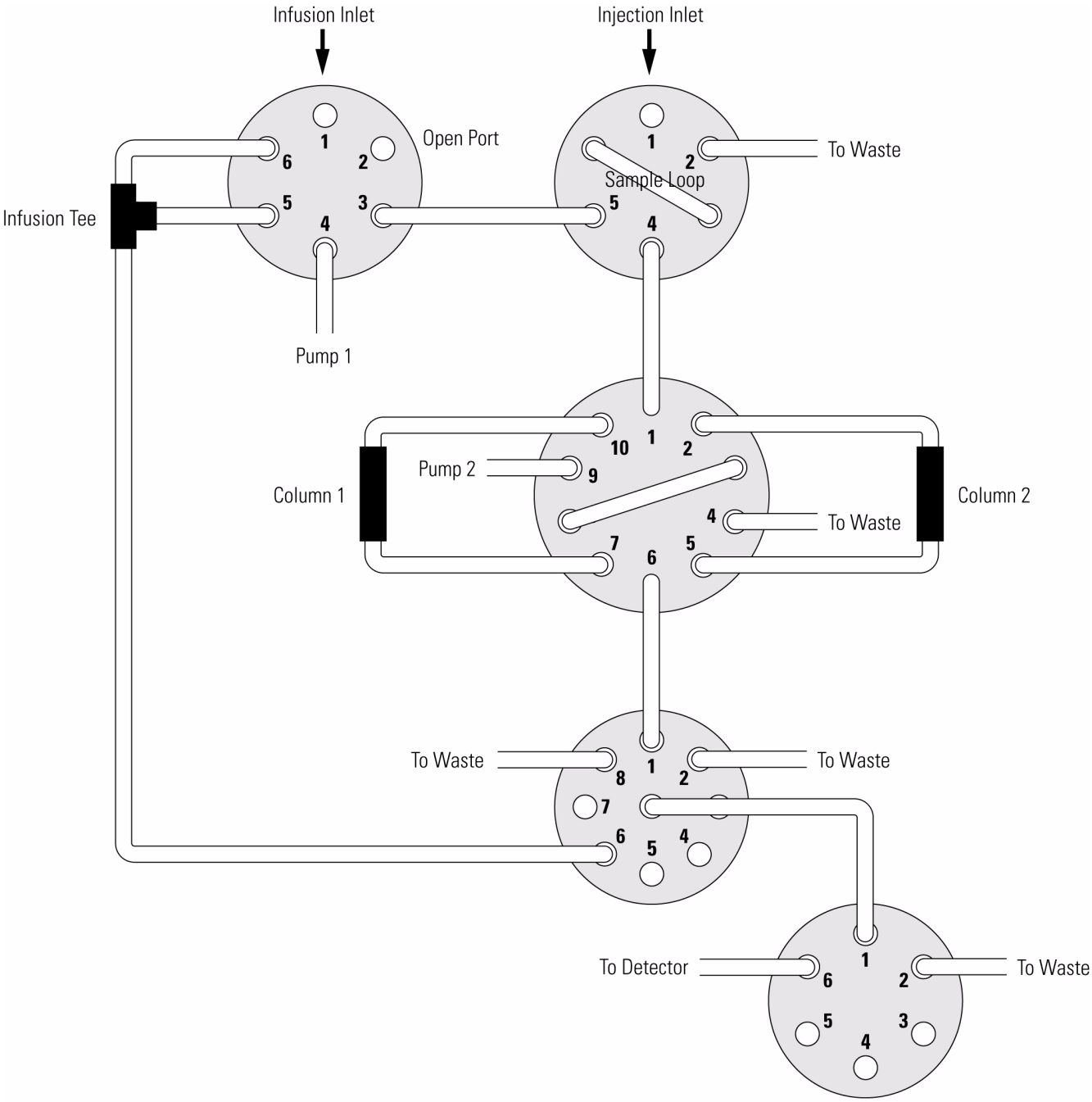
To increase throughput for a gradient analysis, you can set up your LC/MS system in a dual-pump, dual-column configuration and equilibrate one column while performing sample elution with the other column. Figure 48 shows the required configuration.

To alternate columns between consecutive injections, you must use two instrument methods. In the first method, pump 1 produces a gradient for sample elution on the **first** column, and pump 2 produces a gradient that re-equilibrates the **second** column. In the second method, pump 1 produces a gradient for sample elution on the second column, and pump 2 produces a gradient that re-equilibrates the first column.

Using these alternating instrument methods (along with valve switching) allows for each injection to run through a separate column and removes the wait time for column equilibration.

QuickQuan also enables you to use different instrument methods for the acquisition and the optimization.

Figure 48. Injection valve configuration



Using a Macro To Perform Custom Calculations

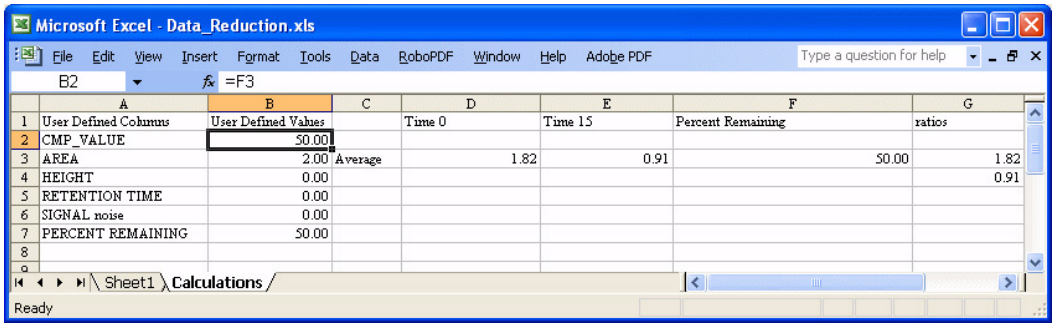
The software includes a Microsoft Excel template file for data reduction, which you can customize to perform the calculations and display the assay results that you require. The location of the Data_Reduction.xls file is as follows:

C:\Xcalibur\QuickQuan\Templates

The Data Reduction template file contains two sheets:

- Sheet 1 in the template is a blank report.
- Sheet 2 is the Calculations page. Figure 49 shows an example.

Figure 49. Example of the Calculations page



	A	B	C	D	E	F	G
1	User Defined Columns	User Defined Values		Time 0	Time 15	Percent Remaining	ratios
2	CMP_VALUE	50.00					
3	AREA	2.00	Average	1.82	0.91	50.00	1.82
4	HEIGHT	0.00					0.91
5	RETENTION TIME	0.00					
6	SIGNAL noise	0.00					
7	PERCENT REMAINING	50.00					
8							

The processing macro Excel file must implement a macro named "RunUserMacro", which QuickQuan "calls" during the data reduction. At a minimum, this macro must recalculate the Calculations page. Setting up the data reduction in this way allows QuickQuan to provide your custom results in real time.

To use the macro for post-processing calculations, you must do both of the following:

- Select the Run User Defined Macros check box when you specify the configuration settings. See "Running an Acquisition" on page 64.
- Select the processing macro template when you select the template files. See "Specifying Template Options" on page 53.

QuickQuan saves the data reduction results in the output path directory.

QuickQuan Views

This appendix describes the primary views that you can display in the QuickQuan window.

Contents

- Compounds Browse View
- Optimization Setup View
- Optimization Tune Report View
- Acquisition Templates View
- Acquisition Setup View
- Acquisition Aria Configuration View
- Acquisition Results Summary View

Compounds Browse View

Use the Compounds Browse view for the following procedures:

- "Defining the Compounds in the Database" on page 11
- "Defining the Drug Sets in the Database" on page 17
- "Viewing Compound and Drug Set Data" on page 20
- "Updating SRM Information" on page 39

In the Compounds Browse view, you can search the compound, drug set, SRM, and source type tables in the currently opened QuickQuan database.

❖ To display the Compounds Browse view

In the QuickQuan navigation pane, click **Compounds**.

The Compounds Browse view has the following controls and parameters.

Control or Parameter	Description
Compound Browser	Displays the table you select in the Table list. The tables are not editable in this view. To edit a table see one of the following procedures: • "Defining the Compounds in the Database" on page 11 • "Defining the Drug Sets in the Database" on page 17 • "Updating SRM Information" on page 39
Table	Specifies one of the following table types for display in the Compound Browser: • "Compounds Table" on page 87 • "Drug Set Names Table" on page 88 • "Source Type Table" on page 89 • "SRM Table" on page 90
Compound	Specifies SQL query commands for filtering the data. To do this, type an SQL statement in the Compounds box, and then click **Query** to filter the data shown in the current table.
Buttons	
<<	Displays the first screen of rows in the displayed table. Use the arrow buttons when the table contains many rows and you want to move around in the table without having to scroll row by row.
<	Displays the previous screen of rows in the displayed table.
>	Click this button to see the next screen of rows in the displayed table.
>>	Click this button to see the last screen of rows in the displayed table.
Query	Filters the data in the currently displayed table using the contents of an SQL statement in the Compound box.

Control or Parameter	Description
Add Compounds	Opens the Add Compounds dialog box, which you use to add and edit compound information in the database or delete compounds from the database. See "Defining the Compounds in the Database" on page 11.
Add Drug Sets	Opens the Add Drug Sets dialog box, which you use to add and edit drug set information in the database or delete drug sets from the database. See "Defining the Drug Sets in the Database" on page 17.
Update SRM Info	Opens the Update SRM Information dialog box. See "Updating SRM Information" on page 39.

Compounds Table

❖ To view the contents of the Compounds table

1. In the QuickQuan navigation pane, click **Compounds**. The Compounds Browse View appears.
2. In the Table box, select **[COMPOUNDS]**.

The Compounds table contains information about how to tune each compound in the QuickQuan database. To modify the Compounds table, use the Add Compounds dialog box. See "Defining the Compounds in the Database" on page 11.

The Compounds table contains the following information for each compound in the database:

Parameter	Description
Compound Name	Name of a compound in the database. To add or delete a compound name, use the Add Compounds dialog box.
Parent Mass	Monoisotopic mass for the compound. To specify the parent mass for a compound, use the Add Compounds dialog box.
Polarity	Polarity of the compound: positive, negative, or both. QuickQuan determines the best polarity during optimization, unless you specify a particular polarity in the Configuration Options dialog box.
Charge State	Charge state for the compound: 1 - 10. To select the charge state for a compound, use the Add Compounds dialog box.

Parameter	Description
Num Products	Number of product ions to be acquired for the compound: 1 - 10. To select the number of product ions for a compound, use the Add Compounds dialog box.
Source Type	Ion source type for tuning the compound, where, 0 = untuned 1 = ESI 2 = APCI 3 = APPI 4 = H-ESI To specify the ion source type for tuning a compound, use the Configuration Options dialog box.

Drug Set Names Table

❖ **To view the contents of the Drug Set Names table**

1. In the QuickQuan navigation pane, click **Compounds**. The Compounds Browse View appears.
2. In the Table box, select **[DRUGSETNAMES]**.

The Drug Set Names table contains the drug sets that you can combine for a given sequence or tune vial. You can group multiple compounds by selecting the compounds under a common drug set name. You can associate up to 10 compounds with a single drug set.

To modify the Drug Set Names table, see "Defining the Drug Sets in the Database" on page 17.

The Drug Set Names table contains the following information for each drug set in the database.

Parameter	Description
Compound	Name of the drug set in the database. To add a drug set to or delete it from the database, use the Add Drug Sets dialog box.
[Compound 1 - Compound 10]	Compounds associated with the selected drug set. To add a compound to a drug set, use the Add Drug Sets dialog box.

Source Type Table

❖ To view the contents of the Source Type table

1. In the QuickQuan navigation pane, click **Compounds**. The Compounds Browse View appears.
2. In the **Table** box, select **SOURCETYPETABLE**.

The **Source Type** table contains the information about the compound after it has been optimized. QuickQuan optimizes for a specific source type: ESI, APPI, APCI, or H-ESI. The compound's polarity, tune file name, and the source type used during the optimization are saved to this table.

You cannot modify the Source Type table. QuickQuan updates the Source Type table whenever an optimization run has finished.

The Source Type table contains the following information for each tuned compound in the database:

Parameter	Description
Compound Name	Name of a compound in the database.
Polarity	The true polarity detected after optimization.
Tune File	The tune file (.TSQtune) - named by QuickQuan - that contains the optimized TSQ Tune parameters.
Raw File	The data collected during the real-time tuning.
PDF File	A tune report stored as a PDF file and generated during the real-time tuning.
Source Type	The ion source type used for this compound during optimization, where, 0 = untuned 1 = ESI 2 = APCI 3 = APPI 4 = H-ESI

SRM Table

❖ To view the contents of the SRM table

1. In the QuickQuan navigation pane, click **Compounds**. The Compounds Browse View appears.
2. In the Table box, select **[SRMTABLE]**.

The **SRM** table contains the information about the SRM transitions detected for a given compound during optimization. The table can hold more than one entry for a given compound, depending on the number of transitions selected.

QuickQuan updates the SRM table whenever an optimization run has finished. To modify the SRM table, see "Updating SRM Information" on page 39.

The SRM table contains the following information for each compound in the database:

Parameter	Description
Compound	Name of the compound.
Parent	Detected mass of the parent compound.
Product	Detected product ion mass of the parent compound.
Col Energy	Optimal collision energy of the product ion.
Q1	Peak width setting used during optimization. Q1 is set to 0.2 for H-SRM; otherwise, Q1 is set to 0.7. The Q1 setting is used to set the peak width for ions passed by the Q1 mass analyzer. The lower the peak width setting, the higher the resolution.
Q3	Peak width setting used during optimization. Q3 is always set to 0.7. The Q3 setting is used to set the peak width for ions passed by the Q3 mass analyzer. The lower the peak width setting, the higher the resolution.
Tube Lens	Optimal tube lens offset.
Width	Scan width used during optimization.
Max Intensity	Maximum intensity of the product ion.

Optimization Setup View

You use the Optimization Setup view to set up compound optimization. See "Setting Up for Optimization" on page 24.

QuickQuan uses the information specified in a tune plate to optimize all the compounds within the plate. The compound information is passed to the TSQ tune application in real time, and QuickQuan monitors the status of each compound during the optimization. The data returned from the optimization is added to the central database. The optimization data for each compound stored in the QuickQuan database includes polarity, tube lens offset, parent ion mass, product ion mass(es), collision energy, tune status report, and tune .raw data.

Note The instrument methods for optimization can differ from the instrument methods for acquisition.

Tip If your system includes a Thermo PAL autosampler with multiple injection ports, multiple valves, and a stream selector, you can speed up the optimization process. See "Bypassing the LC Column and the Dual-Pump, Dual-Column Configuration" on page 81.

Note If you are using the LC column and the tune operation has a time-out before the compounds have been tuned, use a longer delay for the divert valve setting.

❖ To display the Optimization Setup view

In the QuickQuan navigation pane, click **Optimization**, and then click **Setup**.

The Optimization Setup view has the following parameters.

Parameter	Description
Tune and Method Files	
Tune File	Specifies the unoptimized *.TSQTune file to use for this tune plate, for example: C:\Xcalibur\QuickQuan\Templates\ Tune template.TSQTune If you are only acquiring data and not optimizing, a tune file is not necessary.

Parameter	Description
Tune Pos. LC Method	Specifies the instrument method (.meth) file for positive polarity, for example: C:\Xcalibur\QuickQuan\Templates\Tune_LC_Pos.meth You can select different instrument methods for positive and negative tuning when doing multiple injections.
Tune Neg. LC Method	Specifies the instrument method (.meth) file for negative polarity, for example: C:\Xcalibur\QuickQuan\Templates\Tune_LC_Neg.meth You can select different instrument methods for positive and negative tuning when doing multiple injections.
PDF/RAW Output Path	Specifies the folder where the tune status report (PDF file) and tune sample data (.raw file) are stored.
Optimization Settings	
Min. Intensity Threshold	Specifies the intensity thresholds for the product ions. If a compound fails the threshold, the system skips that compound's optimization and goes to the next compound in the list. Range: 500 - 1000000
H-SRM	Activates tuning for H-SRM (precursor ion peak width = 0.2 amu). The H-SRM mode is either turned on or turned off for the entire tune plate. Compounds tuned in H-SRM keep their H-SRM parameters during data acquisition. **Note** When H-SRM is selected, the Adjust Parent Mass option in the Quantum Tune Master [*ion source*] EZ Workspace is also selected. The TSQ Quantum adjusts the parent mass to the resolution of the mass spectrometer. This adjustment might result in a different parent mass being stored in the QuickQuan database than the one you originally specified for the compound. Clear this check box to specify tuning for unit resolution (precursor ion peak width = 0.7 amu).

Parameter	Description
Use Autosampler Infusion During Optimization	Specifies that a flow injection (infusion) of a single sample be used for optimization. See "Bypassing the LC Column and the Dual-Pump, Dual-Column Configuration" on page 81. Clear this check box (default) if you want multiple injections of the same sample. Injections are made for positive and negative polarities, tube lens offsets, product ion masses, and collision energies. **Tip** Selecting the check box can provide faster optimization times.
Inj Volume (ul)	(Use Autosampler Infusion During Optimization option only) Specifies the sample amount to inject for each compound being optimized. The flow rate for the infusion with the Inj Volume determines how long the infusion sample is present during the tuning session. Range: 0 - 500 uL
Plate Setup	
Plate Type	Specifies either the 96-well or 384-well plate type.
Autosampler Tray Name	Specifies the autosampler tray that contains the compounds to be optimized.
Tune Plate graphic	Specifies the layout of the tune plate. Click any well position in this graphic, and then use the Drug Set Selector to associate a drug set with the well. The selected well positions on the Tune Plate graphic are color-coded: • **Green:** Compounds in the drug set have been tuned for this ion source. • **Yellow:** Compounds in the drug set have been tuned for an ion source other than the currently selected ion source. • **Red:** At least one compound in the drug set has not been tuned.
Clear Plate	Clears all wells in the plate of their drug sets.
Clear Well	Clears the selected well of its drug set.

Parameter	Description
Import	Displays the Open dialog box, which you use to import a drug set information file (.txt file). See "Importing Drug Sets Using a Text File" on page 19.
Losses / Adducts	Opens the Losses/Adducts dialog box, which you use to specify that QuickQuan does the following: • Disallows product ion losses that are not very specific. The choices are H2O, NH3, CH3, and two user-definable losses. • Selects adducts. The choices are M+H, M+Na, M+NH4, and three user-definable adducts for positive ions; M-H, M-COO, and three user-definable adducts for negative ions.
Drug Set Selector	
Current Well	Displays the position of the well you selected in the Tune Plate graphic. If the drug set contains only one compound, then the compound name and mass are also displayed.
Drug Set List	Displays all drug sets that you added or imported in the database.
Apply	Associates the selected drug set with the selected well.

Optimization Tune Report View

You can use the Optimization Tune Report view to do the following:

- View a tune results report (PDF file). See "Viewing the Optimization Results" on page 36.
- Open Xcalibur Qual Browser to see the display of the raw data results for the selected compound.

The tune report includes tune status, breakdown curves, and MS/MS spectra.

❖ To display the Optimization Tune Report view

In the QuickQuan navigation pane, click **Optimization**, and then click **Tune Report**.

The Optimization Tune Report view has the following parameters.

Parameter	Description
Compound List	Specifies the compound for which you want to view tune results.
Tune Report text pane	(Read-only) Displays the Quantum Tune Master optimization report (PDF file) for the selected compound. You can view, save, and print this report.
Refresh	Refreshes the Tune Report text pane. QuickQuan automatically updates the display.
Qual Browser	Starts Xcalibur Qual Browser and loads the sample data (.raw file) collected for the selected compound after the compound has been optimized. The .raw data file is stored in the PDF / RAW output path (Export Directory) that you selected in the "Optimization Setup View" on page 91.

Acquisition Templates View

Use the Acquisition Templates view to select the template files that QuickQuan uses to establish the starting conditions for an assay and to specify internal standards, if applicable.

See "Specifying Template Options" on page 53.

❖ To display the Acquisition Templates view

In the QuickQuan navigation pane, click **Acquisition**, and then click **Templates**.

The Acquisition Templates view has the following parameters.

Parameter	Description
Template Information	
Generic Instrument Method	Specifies the file path of the instrument method (.meth file) for the automated analysis. QuickQuan uses the generic instrument method, along with optimized settings from the optimization, to build the complete instrument method for the assay. To create a generic instrument method, see "Creating a Generic Instrument Method" on page 44. Example .meth files are in the following folder: C:\Xcalibur\QuickQuan\Templates
Generic Processing Method	Specifies the file path for the processing method (.pmd file) for automated batch analysis. The generic processing method contains a defined set of parameters that provide QuickQuan with a recipe for automatic quantitation. To create a generic processing method, see "Creating a Generic Processing Method" on page 47. Example .pmd files are in the following folder: C:\Xcalibur\QuickQuan\Templates

Parameter	Description
Processing Macro Template	Specifies the Microsoft Excel template file (.xls) that was designed to invoke a macro automatically. You can use macros to perform custom manipulations of the data acquisition results. See "Using a Macro To Perform Custom Calculations" on page 83. **Note** In addition to selecting the processing macro template, you must select the Run User Defined Macros check box in the Configuration Options dialog box to perform the data reduction.
Output Path	Specifies the folder in which QuickQuan stores the data and template files for an acquisition (for example, .raw, .meth, .pmd, .sld, and PDF files). QuickQuan downloads files for processing to the Xcalibur data system.
Internal Standard	
Use Internal Standard	Activates the internal standard (ISTD) selections. If you select the check box, you must specify a compound for at least one of the following: • Positive ISTD Default • Negative ISTD Default The ISTD lists contain all the compounds in the QuickQuan database.
Positive ISTD Default	Specifies the compound to be used as the positive internal standard. When QuickQuan creates the instrument and processing methods, it uses the positive ISTD compound as a reference for drug sets that contain positive compounds.
Negative ISTD Default	Specifies the compound to be used as the negative internal standard. When QuickQuan creates the instrument and processing methods, it uses the negative ISTD compound as a reference for drug sets that contain negative compounds.

Parameter	Description
Additional Internal Standards	Specifies any target compound for which you want to use an ISTD reference that is different from the negative and positive ISTD defaults. • Target Compound: Specifies the compound for which you want to use an ISTD reference that is different from the defaults. • ISTD Reference: Specifies the ISTD compound to be used as a reference for the corresponding target compound. To specify a compound or ISTD, click the table cell, and then select the compound from the list. When QuickQuan creates the instrument and processing methods, it uses each additional ISTD compound as a reference for the corresponding target compound specified in the table. If a positive or negative ISTD default is not specified, QuickQuan uses the first ISTD from the Additional Internal Standards table as the default.

Acquisition Setup View

Use the Acquisition – Setup view to create an acquisition sequence containing unknown samples, calibration standard samples, quality control samples, and blank samples.

See the following procedures:

- "Creating a Sequence in the Acquisition Setup View" on page 55
- "Importing a Sequence" on page 58

❖ To display the Acquisition Setup view

In the QuickQuan navigation pane, click **Acquisition**, and then click **Setup**.

One row of the sequence corresponds to one sample injection. Each sample is defined by the settings in the corresponding row. Alternatively, you can manually inject samples from the front panel injector, as predefined in the sequence.

For quantitative analysis, a sequence can be generated semi-automatically based on a processing method. For example, Sequence Setup can divide up a large number of samples into smaller groups that are bracketed by calibration sets. The number of calibration levels in each calibration set is defined by the processing method, which you create in Xcalibur Processing Setup. Calibration sets can be shared between brackets to make overlapping brackets, if required. QuickQuan supports sequences with open brackets.

The sequence table parameters include the following.

Parameter	Description
New Sequence	Specifies the start of a new acquisition sequence.
Drug Set	Specifies which drug set is associated with the acquisition sequence. To select a different drug set, click the cell and select from the list.
Sample Name	Displays the name that you assign to your sample. To change a sample name, type the new name in the table cell.

Parameter	Description
Sample Type	Displays the type of sample described by the Sequence row. Different sets of sample types are presented for different bracket types. The sample type defines how Xcalibur processes the sample data. Each sample must be classified as one of the following Xcalibur sample types: • Unknown • Blank • QC (quality control) • Standard Clear • Standard Update To change the sample type, click the cell, and then select a sample type from the list.
Level	For calibration or quality control (QC) samples only, displays the name of the level. To select a different level name, click the cell and select from the list.
Sample ID	Specifies a unique identification (ID) number for each sample. To change the current ID number, type the new ID number in the table cell. **Tip** To edit this field after it is saved, select the cell and press F2. Xcalibur places a cursor at the right side of the cell text. You can then delete the old Sample ID and enter the new Sample ID.
Instrument Method	Specifies the file path and file name of the instrument method (.meth file extension) that defines the acquisition. To select a different method, double-click the right end of the table cell. In the Select Instrument Method dialog box, select the .meth file, and then click **Open**. To create a method, see "Creating a Generic Instrument Method" on page 44.
Vial Position	Specifies the position in the autosampler. To change the position, type the new position in the table cell.

Parameter	Description
Injection Volume	Specifies the injection volume in microliters of sample to be injected. To change the volume, type the new volume in the table cell. If you are using an autosampler, you can set the default injection volume in the Autosampler dialog box in the Instrument Setup window. The minimum and maximum injection volumes that you can use depends upon the autosampler you select. The usable range is dependent upon the injection mode and can be smaller than the range displayed in the status bar. For more details, consult your autosampler manual.
Comment	Displays any comments that you have entered about the sample. Type in the table cell to enter more comments.
Dilution Factor	Displays the dilution factor that was used to prepare the sample. To change this factor, double-click the table cell and type the correct factor. Valid range: 0.001 to 1000.000 If you have specified a processing method for the current Sequence, Xcalibur automatically enters the Dil Factor value from the processing method settings.

Parameter	Description
ISTD Correction Amount	Specifies the correction amount for the internal standard. If the value is not 0.000, the value is used in an algorithm to correct for the case in which the ISTD amounts in the active processing method are correct, but the ISTD amount in one or more samples is different from the specified amount. This correction eliminates the necessity of remaking the samples to the internal standard concentrations or amounts specified in the processing method and re-running the samples. For each component defined as an ISTD, a bulk adjustment factor may be applied to the base response of each ISTD defined in the processing method. • If no correction is required, confirm that a value of 0.000 is entered in the ISTD Corr Amt cell. • If a correction is required, enter the sum of all ISTD amounts or concentrations actually in the sample into the ISTD Corr Amt cell requiring adjustment. The value entered should use the same units as specified in the processing method. Do not type the units, for example, type 20 not 20 ng.
Sample Volume	Displays the volume of a component that has been placed in the sample. The unit for this volume is specified in the Processing Setup window and is only included in Xcalibur reports. Xcalibur does not convert units. To change the sample volume, double-click the table cell and type the correct value. If you have specified a processing method for your sequence, Xcalibur automatically enters the units for the sample volume of the calibration and QC samples from the processing method settings.

Parameter	Description
Sample Weight	Displays the amount of a component that has been placed in the sample. The unit for this volume is specified in the Processing Setup window and is only included in Xcalibur reports. Xcalibur does not convert units. To change the sample weight, double-click the table cell and type the correct value. If you have specified a processing method for your sequence, Xcalibur automatically enters the sample weights of the calibration and QC samples from the processing method.
Processing Method	Specifies the file path and file name of the processing method (.pmd file extension), which tells QuickQuan how to process the raw data. To select a different method, double-click the right end of the table cell. In the Select Processing Method dialog box, select the .pmd file, and then click **Open**. To create a method, see "Creating a Generic Processing Method" on page 47.
Cal File	Specifies a calibration curve file (.xcal), rather than having QuickQuan create one. To specify a calibration file, double-click the right end of the table cell. In the Select Calibration File dialog box, select the .xcal file, and then click **Open**.

Parameter	Description
File Name	QuickQuan automatically creates the file names for the acquired sample data. The file name is a combination of the base file name prefix assigned to a sequence and a sequential sequence number. • If the New File Template is used to create a sequence, the base file name and the sequence starting number are defined at that time. • If the default sequence starting number 1 is not changed, the suffix number is the same as the row number of the sequence, for example, 001, 002, and so on. • If the default sequence starting number is changed to another number, the first sample has the starting number and subsequent rows in the sequence increment by 001. For example, if the starting number is 100, the file name for the first sample has a suffix of 100, the second sample has a suffix of 101, and so on.

Acquisition Aria Configuration View

The Aria Configuration view is available in the Acquisition section only if Aria OS is installed on the computer. You can use QuickQuan with Aria OS to increase the throughput of the acquisition. For an overview of how to use QuickQuan with Aria OS, see the *QuickQuan and Aria OS Quick Start*.

Use the Aria Configuration view to specify the default autosampler (AS) methods and LC methods for the Aria system. You can also specify method and LC system overrides for the individual sequences.

❖ To display the Aria Configuration view

In the QuickQuan navigation pane, click **Acquisition**, and then click **Aria**.

The Aria Configuration view contains the following controls.

Control	Description
Default AS Method	Specifies the AS method (.tmt file extension) for Aria OS to use if no AS method is specified. To specify method, click ... . In the Open dialog box, select the .tmt file, and then click **Open**.
Default LC Method	Specifies the LC method (.htc file extension) for Aria OS to use if no LC method is specified. To specify method, click ... . In the Open dialog box, select the .htc file, and then click **Open**.
Available LC Systems	Displays the status of the LC Systems. If a system is unavailable, the label appears grayed. To change the availability of an LC System, see the *Aria OS User Guide*.
Use Batch Overrides	Activates the Batch Overrides table. If activated, the software uses the specified overrides for the methods and LC systems. If not activated, the software uses the defaults.

Control	Description
Batch Overrides Table	
Drug Set	Displays the drug set name for each sequence. The sequence row number from the "Acquisition Setup View" on page 99 also appears.
AS Method	Specifies a method to override the default AS method for the sequence. To specify an override, click the table cell. In the Open dialog box, select the .tmt file, and then click **Open**. **Note** By default, the AS and LC methods are stored in the Aria Data folder.
LC Method	Specifies a method to override the default LC method for the sequence. To specify an override, click the table cell. In the Open dialog box, select the .htc file, and then click **Open**.
LC1 to LC4	Specifies the LC systems for each sequence. To change the LC systems for a sequence, select or clear the **LC** check boxes in the corresponding row.

Acquisition Results Summary View

Use the Acquisition Results Summary view to display and review the quantitation results.

See "Reviewing Quantitation Results" on page 73.

❖ To display the Acquisition Results Summary view

In the QuickQuan navigation pane, click **Acquisition**, and then click **Results Summary**.

The Acquisition Results Summary view has the following parameters.

Parameter	Description
Results	
Root Directory	Specifies the folder that contains the results, for example: *<your_output_path_directory><timestamp_directory_for_selected_acquisition>*
Combined Sequence	Creates an acquisition sequence (.sld file) that combines all sequences (drug sets) in the assay.
Refresh	Refreshes the Results table.
Qual Browser	Starts Xcalibur Qual Browser and loads the raw data collected in the acquisition.
Quan Browser	Starts Xcalibur Quan Browser and loads the raw data collected in the acquisition.
Results Table	
Sequence Name	Lists the individual acquisition sequence files (.sld) that make up the combined sequence.
Date	Lists the date QuickQuan ran the sequences.
Results	Lists the number of samples in a sequence that were run successfully (Yes) or unsuccessfully (No).
Path	Lists the output directory path in which QuickQuan stores the data and template files for the acquisition (for example, .raw, .meth, .pmd, .sld, and PDF files).

QuickQuan Menus and Toolbar Reference

This appendix provides a reference to the QuickQuan menus, toolbar, and status bar.

Contents

- Acquisition Menu
- File Menu
- Help Menu
- Reports Menu
- View Menu
- Status Bar and Toolbar

Acquisition Menu

The Acquisition menu contains the following commands.

Command	Description
Go	Opens the Configuration Options dialog box, which you use to start the optimization or acquisition. See "Running the Optimization" on page 32 or "Running an Acquisition" on page 64.
Stop	Stops the run of the current optimization or acquisition.
Configuration	Opens the Configuration Options dialog box, which is where you set configuration options.

File Menu

The File menu contains the following commands.

Command	Description	Keyboard Shortcut
New	Populates the QuickQuan views with the default settings, which you can use to create a QuickQuan assay file (.aql).	Ctrl+N
Open	Displays the Open dialog box, which you can use to open a saved QuickQuan assay file (.aql).	Ctrl+O
Save	Saves any changes to the current (open) QuickQuan assay file (.aql).	Ctrl+S
Save As	Opens the Save As dialog box, which you can use to save a new or changed QuickQuan assay file (.aql) with a new file name.	
Open Database	Opens the Select Data Source dialog box, which you use to create or choose file data sources and machine data sources. See "Selecting QuickQuan Data Sources and Databases" on page 3.	
Import Acquisition Sequence – From File	Displays the Open dialog box, which you use to import an acquisition sequence as a sequence file (.sld) or a text file (.txt or .csv). See "Importing a Sequence" on page 58.	
Import Acquisition Sequence – From Template	Opens the Import Sequence Templates dialog box, which you can use to import an acquisition sequence as a sequence template (.sld) plus an Excel template (.xls). See "Importing Excel and Sequence Templates" on page 59	

Command	Description	Keyboard Shortcut
Export Methods	Opens the Export Methods dialog box, which you can use to export methods for use with other applications. You can export the generic instrument method (.meth) and processing method (.pmd) for any drug sets in the QuickQuan database. See "Exporting the Instrument and Processing Methods" on page 70.	
Print	Opens a Print dialog box, which you can use to print the content of the QuickQuan status view.	Ctrl+P
Print Preview	Opens a print preview that displays the first page of the QuickQuan status view in a print format.	
Print Setup	Opens the Print Setup dialog box that you can use to specify print parameters for printing the content of the QuickQuan window.	
[Recently Accessed Files List]	Opens the selected file. Choose the file name of the recently accessed QuickQuan file (.aql) that you want to open.	
Exit	Closes QuickQuan.	

Help Menu

The Help menu contains the following commands.

Command	Description
QuickQuan Help	Displays the Help topics for QuickQuan.
QuickQuan Glossary	Opens the QuickQuan Glossary.
How to Use Online Help	Displays information for using the Help.
About QuickQuan	Opens the About QuickQuan dialog box, which displays information about the QuickQuan version and copyright.

Reports Menu

The Reports menu contains the following commands.

Command	Description
Optimization Summary Report	Opens the Browse for Folder dialog box, which you use to specify a location for the optimization summary report. QuickQuan generates the report automatically in a Microsoft Excel file (.xls). The report shows the compound information that was collected during the optimization of the compounds in the current tune plate. See "Generating an Optimization Summary Report in Excel" on page 39.
Acquisition Summary Report	Opens the Browse for Folder dialog box, which you use to specify a location for the acquisition summary report. The location is *<your_output_path_directory><timestamp_directory_for_selected_acquisition>* QuickQuan generates the report automatically in a Microsoft Excel file (.xls). The report concatenates every summary report for each sequence of the assay into a single acquisition summary report. See "Generating and Viewing the Acquisition Summary Report" on page 76.

View Menu

The View menu contains the following commands.

Command	Description
Toolbar	Displays or hides the QuickQuan Toolbar.
Status Bar	Displays or hides the QuickQuan Status bar.

Status Bar and Toolbar

The QuickQuan window contains a status bar, which appears at the bottom left, and a toolbar at the top of the window below the menus.

- The status bar displays a text description of the menu command or toolbar icon to which the cursor arrow is pointing. If the cursor arrow is pointing to something other than a command or icon (for example, the menu label "File"), the Status Bar displays the text "For Help, press F1".
- The toolbar contains shortcut buttons for the frequently used menu commands.

❖ To show or hide the status bar

Choose **View > Status Bar**.

❖ To show or hide the toolbar

Choose **View > Toolbar**.

The toolbar contains the following buttons.

Button		Description
	New	Populates the QuickQuan views with the default settings, which you can use to create a QuickQuan assay file (.aql).
	Open	Displays the Open dialog box, which you can use to open a saved QuickQuan assay file (.aql).
	Save	Opens the Save As dialog box, which you can use to save a new or changed QuickQuan assay file (.aql) with a new file name.
	Start Acquisition	Displays the Configuration Options dialog box, which you use to start the run of the selected optimization or acquisition. See "Running an Acquisition" on page 64.
	Stop Acquisition	Stops the run of the current optimization or acquisition.

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